Vladas Sidoravičius
Editor

New Trends in Mathematical Physics

Selected Contributions of the 15th International Congress on Mathematical Physics

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Selected Contributions of the XVth International Congress on Mathematical Physics

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Vladas Sidoravičius
Instituto de Matemática Pura e Aplicada (IMPA)
Estrada Dona Castorina 110
Rio de Janeiro, RJ
Brazil
vladas@impa.br

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Preface

The XV-th International Congress on Mathematical Physics took place in Rio de Janeiro, on August 5–11, 2006. I believe it was a very successful and enjoyable meeting. It is very fortunate for our community that Latin America, and especially Brazil, in decades has become the place where all fields of intellectual activity which are traditionally regarded as part of Mathematical Physics are developing with steady pace and remarkable quality. Another important aspect of this development is that besides areas which already have worldwide recognition and long standing tradition in Brazil such as Dynamical Systems, Statistical Mechanics, Probability Theory, etc., there is intensive growth in other directions such as String Theory and Algebraic Geometry. Brazil's major universities and research institutes such as IMPA and CBPF are successfully bringing up a new generation of researchers in our field. Thus it was especially pleasant to see that among more than 500 participants of the Congress, the majority was constituted by young researchers and graduate students.

Given the enormous range of subjects covered during the Congress, and the diversity of scientific contributions, it would be pointless to summarize the contents here—the quality is reflected in these pages.

Traditionally, besides its very intense scientific program, the Congress was the occasion for the award of the Henri Poincaré Prizes of the IAMP, sponsored by the Daniel Iagolnitzer Foundation. The Laureates for the year 2006 were Ludwig Faddeev, David Ruelle and Edward Witten.

As with any other period between successive IAMP Congresses, this one was witnessing scientific excitement and important developments in many areas. Perelman's proof of the Poincaré conjecture and progress in geometrization program were the central topic of many discussions, seminars, talks and meetings. I also would like to mention the spectacular developments in the area of Random Matrices and the progress made by F. Guerra and M. Tallagrand in spin-glasses. Perhaps it would not be an exaggeration to say that the development of Stochastic Schramm-Loewner Evolution and understanding of two-dimensional critical systems and its connections with Conformal Field Theory continue to be one of the most fascinating chapters of contemporary Probability Theory and Statistical Mechanics. A few days

after the Congress in Rio, Wendelin Werner, the plenary speaker of the XVth ICMP, was awarded the Fields medal for his contribution to this field. And in the spring of 2007 Srinivasa Raghu Varadhan, the chair of the International Scientific Committee of the XV ICMP, was awarded the Abel Prize. I believe this speaks not only about the recognition of the increasing role of Probability Theory and appreciation of its mathematical depth, but also about importance of all our community, since research performed by W. Werner and S.R. Varadhan, and the origins of questions they answer, are deeply rooted in the fields of Mathematical Physics.

However it was also the time when with great sadness we learned in September 2008 about the untimely death of Oded Schramm, the inventor of SLE and the 2003 Poincaré Prize recipient.

The preparation of the Congress as usual has taken a huge amount of work. On the scientific side I must thank all the members of the International Scientific Committee. I would like also to express my deep gratitude and affection to David Brydges, the President of International Association of Mathematical Physics during the period 2003–2005, who was the visionary, driving force and first aid help at all occasions. Among the local organizers I have to single out first of all Prof. J.F. Perez and Profs. C. Camacho, J. Palis and M. Viana who were pivotal for the success of the meeting. And last but no least, all my thanks and appreciation to the whole team of logistic and administrative support of DAC, masterfully conducted by Mme. S. Lima.

The Congress could not have happened without the generous support of numerous sponsors and efforts of many individuals, who are listed on the homepage of the congress (http://www.iamp.org/). I'm most grateful to them all. The reader also will find there the list of participants of the meeting.

Finally a few words on the organization of the book. We were not seeking to produce a standard "Proceedings" book. To document the content of the plenary talks and invited talks in all specialized sessions, in the Appendix to the book we include the abstracts of the meeting as they stood in August 2006, so that the interested reader can trace back the contents of all talks. As for the main part of the book, we invited all plenary speakers and invited speakers of specialized sessions to contribute with articles that they find appropriate for this volume, reflecting the current state of the art in Mathematical Physics, and which are written according to their own vision of the development of their fields. Thus, as a result, the reader will find here the original research articles, extensive reviews, as well as extended versions of talks.

Vladas Sidoravičius

Foreword

Mathematical Physics has on occasion weathered the label of being a curious subset of Theoretical Physics confined to "esoteric" questions such as exchanges of limits, measurability of sets, existence of solutions to equations, in other words, an obsession with issues that deserve little or no mention at all. In my view this is a destructive attitude and it has to be made clear that the distinction should be, and is, between *interesting* and *not interesting* or *physically relevant* and *irrelevant* and that there is a virtue in the clear formulation of problems and a clear distinction between assumptions and results.

It is a fact that these goals have not generated any damage to research, as the main and best known contributions to Physical theories prove (Ptolemaic and Copernican astronomy, Keplerian and Newtonian mechanics, ergodic hypothesis, electromagnetism, relativity, quantum mechanics, condensed matter, quantum field theory, stability of matter, symmetries in atomic and particle Physics, ...): the key works, even when not formulated in mathematical terms, have always kept an extremely lucid distinction between assumptions and consequences and have been influential and recognized by all.

Nevertheless the above mentioned attitudes have led to problems that inevitably generate difficulties in jobs hiring, obtaining grants, priority recognition, impact factor comparison, and more: so that IAMP has the scope of helping the rather large community that looks at problems and subjects their analysis to rigorous criticism. In the end this amounts to a distinction between hypotheses, deductions and results when reading the "book of Nature", which is recognized by all of us, with Galilei and his predecessors and followers, to be written in mathematical characters.

The ICMP's meetings have been designed to inform all of the IAMP members of the status of our work, to provide to the entire Physics community evidence of the relevance of the results and to show the close interest that we pay to the evolution of Theoretical Physics.

The Rio meeting is the most recent example of the width of the interests and the open mindedness of its members. A glimpse at the conference titles shows that the most varied subjects have been presented in the plenary talks and in the parallel sessions. From geometry, to string theory, to general relativity, to statistical

mechanics in equilibrium (classical and quantum) and nonequilibrium fluctuations, to dynamical systems, to symmetries, to PDE's ....

The three *Henri Poincaré prizes*, that the Iagolnitzer Foundation sponsors and the IAMP awards, recognize exceptional contributions and honor three colleagues, for their great contributions to Physics and for providing examples that we will try to imitate on how to look at problems that we cherish.

We think that the wide variety of session and plenary talks will provide, through the publication of the present proceedings, inspiration for new challenging problems, and confidence, to the many young colleagues who want to continue the exciting experience of those of us who have followed the developments from the early '960's and can feel the immense difference between what was known at the time and today.

Finally IAMP thanks the local organizers of the meeting in Rio for the effort they made to make easy and agreeable participation by our colleagues, particularly those who undertook a long journey to attend our meeting.

It has been decided that ICMP09 will be held in Prague and we are sure that it will continue the tradition of excellence that this and earlier ICMP meetings have bequeathed to us.

Giovanni Gallavotti
IAMP President 2006–2008

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The XV International Congress on Mathematical Physics was organized by the International Association of Mathematical Physics (IAMP), in association with Instituto Nacional de Matemática Pura e Aplicada (IMPA), Rio de Janeiro, Instituto do Milênio (IM-AGIMB) and Petrobras (Brazil).

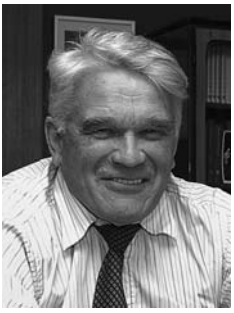
Past Congresses

Moscow (Russia), 1972
Warsaw (Poland), 1974
Kyoto (Japan), 1975
Roma (Italy), 1977
Lausanne (Switzerland), 1979
Berlin (Germany), 1981
Boulder (USA), 1983
Marseille (France), 1986
Swansea (United Kingdom), 1988
Leipzig (Germany), 1991
Paris (France), 1994
Brisbane (Australia), 1997
London (United Kingdom), 2000
Lisbon (Protugal), 2003

The Henri Poincaré Prize

The Henri Poincaré Prize is awarded by the International association of Mathematical Physics (IAMP) and is sponsored by Fundation Culturelle Daniel Iagolnitzer (Paris). The 2006 Laureates were Ludwig Faddeev (Russia), David Ruelle (France), Edward Witten (USA).

Ludwig Faddeev



For his many deep and important results to the theory of quantum fields, quantization of non-commutative gauge theories, scattering in quantum mechanics and quantum field theory, and the theory of integrable systems.

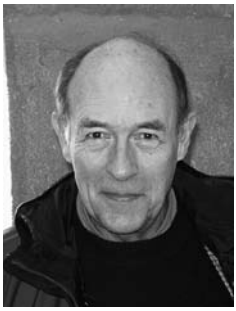
Laudatio by Professor F. Smirnov

It would be not enough to say that Ludwig Dmitrievich Faddeev works in the field of mathematical physics. Rather he is one of the creators of modern mathematical physics. In the late fifties when he started his scientific career, different branches of what we now call mathematical physics were essentially unrelated. It should be taken into account, for example, that at that time Quantum Mechanics was younger than String Theory is today. For me the main feature of Faddeev as a scientist is his belief that mathematical beauty is the most important guiding principle in physics.

For that reason I consider him as a great idealist. Certainly Faddeev had predecessors who shared the same point of view. He himself cites in that respect P.A.M. Dirac, H. Weyl and V.A. Fock. Our generation takes many things for granted. We know that Quantum Mechanics is a deformation of Classical Mechanics, we understand the importance of Hamiltonian Methods in that respect, we know that the functional integral is not just a fancy idea of Feynman but an important tool in Quantum Field Theory, that geometry plays a role in Quantum Field Theory along with the theory of Lie groups, that classical nonlinear equations admit non-trivial solutions which give rise to new particles after quantization, and hence it is not necessary for every particle to correspond to its own field. All that was taught to us, but for Faddeev this was a result of personal development. He had to understand all these matters himself and often in a hostile environment. That is why he understands them deeper than we do. Let me describe the main works of Faddeev. He started with the study of Quantum Mechanics in the framework of functional analysis as was usual at the time. The PhD thesis of Faddeev is devoted to the inverse problem for one-dimensional Schrödinger operator. Profound knowledge of the subject turned out, much later, to be of central importance in relation to the Korteweg-deVries equation. I think the main discovery of his early work was the recognition of the importance of functional determinants. I remember, at a later point, when I was surprised that the formulae for the form factors in integrable models are given by determinants, Faddeev told me: "Solution to any good problem is given by a determinant." Certainly, this was a joke, but it is true that we find several remarkable determinants in Faddeev's works. Then comes the three body problem with the famous Faddeev's equations. This work combines an elegant original idea with very sophisticated techniques. Faddeev himself considered this work as a mathematical solution of a difficult physical problem. Actually its importance is much wider: all computer calculations needed for applications today are done using Faddeev's equations. The sixties was a period of very diverse and successful scientific activity for Faddeev. It is difficult to establish an exact chronology because at that time he was working very actively in many different fields. For an ordinary person it would be impossible to deal with such different matters simultaneously. I have already said that I consider mathematical beauty as the main source of Faddeev's inspiration in physics, but the opposite is also true: believing that physics is described by beautiful mathematics he naturally comes to the conclusion that a good problem in physics must provide new insight into pure mathematics. A realization of this idea is presented by his remarkable derivation of the Selberg trace formula by the methods of scattering theory. Determinants once again! The theory of automorphic functions is so far from his original area that once again he had to understand the subject by himself, and it is impressive how deep and clear this understanding is. Yet another work from the same period concerns the three-dimensional inverse problem. In all the years that followed very little was added to Faddeev's work on the subject, and it remains a rare example of elegance in mathematical physics. Now comes the jewel of the scientific career of Faddeev: quantization of the Yang-Mills theory. I remember long ago C. Itzykson told me: "We were doing the usual perturbation theory, Faddeev taught us the functional integral." I think this is the main discovery of Faddeev in Quantum Field Theory: the

functional integral and the measure of integration in it should be taken seriously. This discovery led him (with V.N. Popov) to the discovery of one more determinant which will surely stay in Quantum Field Theory forever. In the seventies Faddeev was one of the first to recognize the importance of the newly discovered solutions of non-linear PDE—solitons. He was not interested in applications to hydrodynamics, rather to Quantum Field Theory, being convinced that solitons would allow for the reduction of the number of fields in Lagrangians. The program which he developed with his colleagues and students was logically clear: to develop the Hamiltonian approach as the first step towards quantization, to find integrable relativistic models, to perform semi-classical quantization, to quantize exactly. All this was done during the seventies-eighties. As a result, unexpected connections have been found with works by H. Bethe, C.N. Yang, R. Baxter, and an entire new field of mathematics, the theory of Quantum Groups, appeared. In the early seventies Faddeev started to look for multidimensional solitons. He returned to this problem and to Yang-Mills theory in the nineties, and has been working in this direction up till the present time. I wish him many new achievements and I hope everybody will join me in echoing this sentiment. Congratulations Ludwig Dmitrievich!

David Ruelle



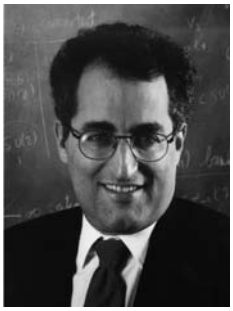
For his outstanding contributions to quantum field theory, both classical and quantum statistical mechanics, and dynamical systems theory.

Laudatio by Professor G. Gallavotti

Professor David Ruelle's scientific carrier is remarkable for his various contributions and for the conceptual continuity of the development through them. He has been among the first to realize the relevance of a rigorous derivation of the properties of equilibrium Statistical Mechanics as an essential step towards understanding the theory of phase transitions. His work has been an important guide to the scientists who in the sixties were attempting accurate measurements of thermodynamic quantities, like critical exponents, in various statistical mechanics models using the newly available electronic computational tools in conjunction with the use of rigorous results for assessing the correctness and reliability of the computations. The treatise on Statistical Mechanics, 1969, has become a classic book and it is still the basis of the formation of the new generations of scientists interested in the basic aspects of the theory. He has written several other monographs which are widely known and used. His critical work on the structure of Equilibrium Statistical Mechanics led him to undertake in 1969 the analysis of the theory of turbulence. The first publication on the subject was the epoch making paper "On the nature of turbulence" in collaboration with Takens. The paper criticized the theory of Landau, based on the increasing complexity of quasi periodicity arising from successive bifurcations in the Navier Stokes equations. The main idea that only "generic" behavior should be relevant was a strong innovation at the time: this is amply proved by the hundreds of papers that followed on the subject, theoretical, numerical and experimental. The works making use of Ruelle's ideas stem also, and perhaps mainly, from the innovative papers Ruelle wrote (and continues to write) after the mentioned one. There he developed and strongly stressed the role that dynamical systems ideas would be relevant and important in understanding chaotic phenomena. The impact on experimental works has been profound: one can say that after the first checks were performed, some by notoriously skeptical experimentalists, and produced the expected results we rapidly achieved, by the end of the seventies, a stage in which the "onset of turbulence" was so well understood that experiments dedicated to check

the so called "Ruelle-Takens" ideas on the onset of turbulence were no longer worth being performed as one would know what the result would be. The very fact that a study of the onset of turbulence was physically interesting was new at the time (the sixties). The ideas had been independently worked out by Lorenz, earlier (in a 1963 paper): this became clear almost immediately. However I think that Ruelle's view, besides reviving the interest in Lorenz' work, which had not been appreciated as it should have, were noticed by physicists and mathematicians alike, and perhaps had more impact, because they were more general and ambitious in scope and aimed at understanding from a fundamental viewpoint a fundamental problem. In 1973 he proposed that the probability distributions that describe turbulence be what is now called the "Sinai-Ruelle-Bowen" distribution. This was developed in a sequence of many technical papers and written explicitly only later in 1978. In my view this is the most original contribution of Ruelle: it has not been well understood for years although it has been quoted in impressively many works on chaos. It had impact mostly on numerical works, but it proposes a fundamental solution to one of the most outstanding theoretical questions: what is the analog of the Boltzmann-Gibbs distribution in non equilibrium statistical mechanics? His answer is a general one valid for chaotic systems, be them gases of atoms described by Newton's laws or fluids described by Navier Stokes equations (or other fluid dynamics equations). Today the idea is still a continuous source of works both theoretical and experimental. Since the beginning of his work he has studied also problems concerning other fields like operator theory and operator algebras obtaining results remarkable for originality and depth: I mention here only his results on the LeeYang theorem on the location of the zeros of polynomials (a subject to which he continued to add new results and applications) and the Haag-Ruelle theory of scattering in relativistic quantum fields, very widely studied and applied, which is still today virtually the only foundation for relativistic scattering theory, employed in mathematical Physics, high energy phenomenology and theoretical Physics. In the last few years he has also provided important impulse to the development of non-equilibrium statistical mechanics: his work continues in this direction at the highest level. He has developed foundational papers for the theory of non-equilibrium Thermodynamics particularly with respect to the concept of entropy. The work of Ruelle is of mathematical nature: but it is an example of how important a conceptually rigorous and uncompromising approach can be fruitful and lead to progress in very applied fields like experimental fluid mechanics or numerical molecular dynamics simulations. His work is in the tradition of the 1800's fundamental investigations in Physics. His work, books and papers, is always very careful, clear and polished: every word, however, is important and requires attention. The awarding of the prize recognizes the cultural influence that he has exercised in the last thirty years or so: and we are all here united in this recognition.

Edward Witten



For his work on string theory which laid down the foundation of this subject. His work has been most influential and inspiring also in mathematical subdisciplines like geometry and topology.

Laudatio by Professor A. Jaffe

Edward Witten is in the midst of an enormously productive career as a mathematical physicist. Born in 1951 in Baltimore, he began his undergraduate studies by majoring in history. Edward certainly had the opportunity for prior exposure to sophisticated physics as his father Louis is a noted expert on relativity and gravitation. After his undergraduate studies, Edward returned to physics, working with David Gross at Princeton, and receiving his doctorate in 1976.

Edward's early work left an immediate impression on experts. He discovered a new class of instanton solutions to the classical Yang-Mills equations, very much a central subject at the time. He pioneered work on field theories with N-components and the associated "large-N limit" as N tends to infinity. Three years later as a Junior Fellow at Harvard he had already established a solid international reputation both in research and as a spell-binding lecturer. That year several major physics departments took the unusual step, at the time an extraordinary one, to attempt to recruit a young post-doctoral fellow to join their faculty as a full professor! At that point Edward returned to Princeton with Chiara Nappi, my post-doctoral fellow and Edward's new wife. Edward has been in great demand ever since.

Edward already became well-known in his early work for having keen mathematical insights. He re-interpreted Morse theory in an original way and related the Atiyah-Singer index theorem to the concept of super-symmetry in physics. These ideas revolved about the classical formula expressing the Laplace-Beltrami operator in terms of the de Rham exterior derivative, $\triangle = (d + d^*)^2$. This insight was interesting in its own right. But it inspired his applying the same ideas to study the index of infinite-dimensional Dirac operators D and the self-adjoint operator $Q = D + D^*$, known in physics as super-charges, related to the energy by the representation $H = Q^2$ analogous to the formula for $\triangle$. This led to the name "Witten index" for the index of D, a terminology that many physicists still use.

In 1981 Witten also discovered an elegant approach to the positive energy theorem in classical relativity, proved in 1979 by Schoen and Yau. What developed as

Witten's hallmark is the insight to relate a set of ideas in one field to an apparently unrelated set of ideas in a different field. In the case of the positive energy theorem, Witten again took inspiration from super-symmetry to relate the geometry of space-time to the theory of spin structures and to an identity due to Lichnerowicz. The paper by Witten framed the new proof in a conceptual structure that related it to old ideas and made the result immediately accessible to a wide variety of physicists and mathematicians. In 1986 Witten's had a spectacular insight by giving a quantum-field theory interpretation to Vaughan Jones' recently-discovered knot invariant. Witten showed that the Jones polynomial for a knot can be interpreted as the expectation of the parallel transport operator around the knot in a theory of quantum fields with a Chern-Simons action. This work set the stage for many other geometric invariants, including the Donaldson invariants, being regarded as partition functions or expectations in quantum field theory. In most of these cases, the mathematical foundations of the functional integral representations can still not be justified, but the insights and understanding of the picture will motivate work for many years in the future.

With the resurgence of "super-string theory" in 1984, Witten quickly became one of its leading exponents and one of its most original contributors. His 1987 monograph with Green and Schwarz became the standard reference in that subject. Later Witten unified the approach to string theory by showing that many alternative string theories could be regarded as different aspects of one grand theory.

Witten also pioneered the interpretation of symmetries related to the electromagnetic duality of Maxwell's equations, and its generalization in field theory, gauge theory, and string theory. He pioneered the discovery of $SL(2, Z)$ symmetry in physics, and brought concepts from number theory, as well as geometry, algebra, and representation theory centrally into physics.

In understanding Donaldson theory in 1995 Seiberg and Witten formulated the equations named after them which have provided so much insight into modern geometry. With the advent of this point of view and fueled by its rapid dissemination over the Internet, many geometers saw progress in their field proceed so rapidly that they could not hope to keep up.

Not only is Witten's own work in the field of super-symmetry, string theory, M-theory, dualities and other symmetries of physics legend, but he has trained numerous students and postdoctoral coworkers who have come to play leading roles in string theory and other aspects of theoretical physics.

I could continue on and on about other insights and advances made or suggested by Edward Witten. But perhaps it is just as effective to mention that for all his mentioned and unmentioned work, Witten has already received many national and international honors and awards. These include the Alan Waterman award in 1986, the Fields Medal in 1990, the CMI Research Award in 2001, the U.S. National Medal of Science in 2002, and an honorary degree from Harvard University in 2005. Witten is a member of many honorary organizations, including the American Philosophical Society and the Royal Society. While Witten may not need any additional recognition, it is an especially great personal pleasure and honor, as one of the original founders of IAMP, to present Edward Witten to receive the Poincaré prize in 2006.

Contributors

Michael Aizenman Departments of Mathematics and Physics, Jadwin Hall, Princeton University, P.O. Box 708, Princeton, NJ 08544, USA, aizenman@princeton.edu

Nalini Anantharaman CMLS, École Polytechnique, 91128 Palaiseau, France, nalini@math.polytechnique.fr

Lars Andersson Department of Mathematics, University of Miami, Coral Gables, FL 33124, USA; Albert Einstein Institute, Am Mühlenberg 1, 14476 Golm, Germany, larsa@math.miami.edu

Giuseppe Benfatto Dipartimento di Matematica, Università di Roma "Tor Vergata", Via della Ricerca Scientifica, 00133 Rome, Italy, benfatto@mat.uniroma2.it

Christoph Bergbauer Institut für Mathematik II, Freie Universität Berlin, Arnimallee 3, 14195 Berlin, Germany; Erwin-Schrödinger-Institut, Boltzmanngasse 9, 1090 Vienna, Austria, bergbau@math.fu-berlin.de

Lorenzo Bertini Dipartimento di Matematica, Università di Roma 'La Sapienza', P.le Aldo Moro 2, 00185 Rome, Italy, bertini@mat.uniroma1.it

Mikhail S. Birman Faculty of Physics, St. Petersburg State University, Ulyanovskaya, 3, St. Petersburg 198504, Russian Federation

Pavel M. Bleher Department of Mathematical Sciences, Indiana University-Purdue University Indianapolis, 402 N. Blackford St., Indianapolis, IN 46202, USA, bleher@math.iupui.edu

Martin Bojowald Institute for Gravitational Physics and Geometry, The Pennsylvania State University, 104 Davey Lab, University Park, PA 16802, USA, bojowald@gravity.psu.edu

Stella Brassesco Departamento de Matemáticas, Instituto Venezolano de Investigaciones Científicas, Apartado Postal 20632, Caracas 1020-A, Venezuela, sbrasses@ivic.ve

Todd A. Brun Communication Sciences Institute, Department of Electrical Engineering Systems, University of Southern California, 3740 McClintock Ave., EEB 502, Los Angeles, CA 90089-2565 USA, tbrun@usc.edu

Paolo Buttà Dipartimento di Matematica, Università di Roma 'La Sapienza', P.le Aldo Moro 2, 00185 Rome, Italy, butta@mat.uniroma1.it

Jérôme Buzzi Laboratoire de Mathematique d'Orsay C.N.R.S., Université de Paris-Sud, Orsay Cedex, France, jerome.buzzi@math.u-psud.fr

Federico Camia Department of Mathematics, Vrije Universiteit Amsterdam, De Boelelaan 1081a, 1081 HV Amsterdam, The Netherlands, fede@few.vu.nl

Nicoletta Cancrini Dip. Matematica, Univ. l'Aquila, 1-67100 L'Aquila, Italy, nicoletta.cancrini@roma1.infn.it

Gabriel Lopes Cardoso Arnold Sommerfeld Center for Theoretical Physics, Department für Physik, Ludwig-Maximilians-Universität München, Munich, Germany, gcardoso@theorie.physik.uni-muenchen.de

James Colliander Department of Mathematics, University of Toronto, Bahen Centre, Toronto, Ontario M5S 3G3, Canada, colliand@math.toronto.edu

Lorenzo J. Díaz Departamento de Matemática, PUC-Rio, Marquês de São Vicente 225, Gávea, Rio de Janeiro 225453-900, Brazil, lodiaz@mat.puc-rio.br

Sergio Dain Facultad de Matemática, Astronomía y Física, Universidad Nacional de Córdoba, Ciudad Universitaria, 5000 Córdoba, Argentina, name@email.address

David Damanik Department of Mathematics, Rice University, Houston, TX 77005, USA, damanik@rice.edu

Gesualdo Delfino International School for Advanced Studies (SISSA), via Beirut 2-4, 34014 Trieste, Italy; Istituto Nazionale di Fisica Nucleare, Sezione di Trieste, Italy, delfino@sissa.it

Bernard Derrida Laboratoire de Physique Statistique, Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France, derrida@lps.ens.fr

Igor Devetak Ming Hsieh Electrical Engineering Department, University of Southern California, Los Angeles, CA 90089, USA, devetak@usc.edu

Patrick Dorey Dept. of Mathematical Sciences, University of Durham, Durham DH1 3LE, UK, p.e.dorey@durham.ac.uk

Boris Dubrovin SISSA, via Beirut 2-4, 34014, Trieste, Italy; Steklov Mathematical Institute, Moscow, Russia, dubrovin@sissa.it

Clare Dunning IMSAS, University of Kent, Canterbury CT2 7NF, UK, t.c.dunning@kent.ac.uk

Paul Fendley Department of Physics, University of Virginia, Charlottesville, VA 22904-4714, USA, fendley@rockpile.phys.virginia.edu

L.R.G. Fontes Instituto de Matemática e Estatística, Universidade de São Paulo, Rua do Matão 1010, Cidade Universitária, 05508-090 São Paulo SP, Brasil, lrenato@ime.usp.br

François Germinet Département de Mathématiques, Univ. Cergy-Pontoise, CNRS UMR 8088, IUF, 95000 Cergy-Pontoise, France, germinet@math.u-cergy.fr

Francesco Guerra Department of Physics, Sapienza University of Rome and INFN, Section of Roma 1, Rome, Italy, francesco.guerra@roma1.infn.it

Sergei Gukov Department of Physics, University of California, Santa Barbara, CA 93106, USA, gukov@theory.caltech.edu

Min-Hsiu Hsieh Ming Hsieh Electrical Engineering Department, University of Southern California, Los Angeles, CA 90089, USA, minhsiuh@gmail.com

Arne Jensen Department of Mathematical Sciences, Aalborg University, Fr. Bajers Vej 7G, 9220 Aalborg O, Denmark, matarne@math.aau.dk

Jürg Käppeli Institut für Physik, Humboldt Universität, Berlin, Germany, kaeppeli@aei.mpg.de

Yasuyuki Kawahigashi Department of Mathematical Sciences, University of Tokyo, Komaba, Tokyo, 153-8914, Japan, yasuyuki@ms.u-tokyo.ac.jp

Alexander Kiselev Department of Mathematics, University of Wisconsin, Madison, WI 53706, USA, kiselev@math.wisc.edu

Abel Klein Department of Mathematics, University of California, Irvine, CA 92697-3875, USA, aklein@uci.edu

Axel Kleinschmidt Max Planck Institute for Gravitational Physics, Albert Einstein Institute, Am Mühlenberg 1, 14476 Potsdam, Germany, axel.kleinschmidt@aei.mpg.de; Present address: Service de Physique Théorique et Mathématique, Université Libre de Bruxelles & International Solvay Instititutes, Campus Plaine CP231, Boulevard du Triomphe, 1050 Bruxelles, Belgium, axel.kleinschmidt@ulb.ac.be

Herbert Koch Mathematical Institute, University of Bonn, Beringstraße 1, 53115 Bonn, Germany, koch@math.uni-bonn.de

Oleg Kozlovski Mathematics Institute Zeeman Building, University of Warwick, Coventry CV4 7AL, England, UK, oleg@maths.warwick.ac.uk

Igor Krasovsky Department of Mathematical Sciences, Brunel University West London, Uxbridge UB83PH, UK, Igor.Krasovsky@brunel.ac.uk

Dirk Kreimer CNRS at Institut des Hautes Etudes Scientifiques, 35 route de Chartres, 91440 Bures-sur-Yvette, France; Center for Mathematical Physics, Boston University, 111 Cummington Street, Boston, MA 02215, USA, kreimer@ihes.fr

Antti Kupiainen Department of Mathematics, Helsinki University, P.O. Box 4, 00014 Helsinki, Finland, ajkupiai@mappi.helsinki.fi

Giovanni Landi Dipartimento di Matematica e Informatica, Università di Trieste, Via A. Valerio 12/1, 34127 Trieste, Italy; INFN, Sezione di Trieste, Trieste, Italy, landi@units.it

Elliot H. Lieb Departments of Mathematics and Physics, Jadwin Hall, Princeton University, P.O. Box 708, Princeton, NJ 08544, USA, lieb@princeton.edu

P.H.S. Lima Instituto de Matemática e Estatística, Universidade de São Paulo, Rua do Matão 1010, Cidade Universitária, 05508-090 São Paulo SP, Brasil, plima@ime.usp.br

Marcos Mariño Département de Physique Théorique and Section de Mathématiques, Université de Genève, 1211 Genève 4, Switzerland, marcos.marino@unige.ch

Fabio Martinelli Dip. Matematica, Univ. Roma Tre, Largo S.L. Murialdo, 00146, Rome, Italy, martin@mat.uniroma3.it

Davide Masoero SISSA, via Beirut 2-4, 34014 Trieste, Italy, masoero@sissa.it

Marco Merkli Department of Mathematics and Statistics, Memorial University of Newfoundland, St. John's, NL A1C 5S7, Canada, merkli@mun.ca

Jens Mund Departamento de Física, ICE, Univ. Federal de Juiz de Fora (UFJF), Juiz de Fora, Brazil, mund@fisica.ufjf.br

Giuseppe Mussardo International School for Advanced Studies, Via Beirut 1, 34013 Trieste, Italy; Istituto Nazionale di Fisica Nucleare, Sezione di Trieste, Trieste, Italy, mussardo@sissa.it

Bruno Nachtergaele Department of Mathematics, University of California, Davis, CA 95616, USA, bxn@math.ucdavis.edu

Gheorghe Nenciu Faculty of Physics, University of Bucharest, P.O. Box MG 11, 077125 Bucharest, Romania; Institute of Mathematics of the Romanian Academy, P.O. Box 1-764, 014700 Bucharest, Romania, Georghe.Nenciu@imar.ro

Charles M. Newman Courant Institute of Mathematical Sciences, New York University, New York, NY 10012, USA, newman@courant.nyu.edu

Stéphane Nonnenmacher Institut de Physique Théorique, CEA/DSM/PhT, Unité de recherche associée au CNRS, CEA/Saclay, 91191 Gif-sur-Yvette, France, snonnenmacher@cea.fr

Stefano Olla Ceremade, UMR CNRS 7534, Université de Paris Dauphine, Place du Maréchal De Lattre De Tassigny, 75775 Paris Cedex 16, France, olla@ceremade.dauphine.fr

Enrique R. Pujals IMPA, Estr. Dona Castorina 110, CEP 22460-320, Rio de Janeiro, R.J., Brazil, enrique@impa.br

Cyril Roberto L.A.M.A., Univ. Marne-la-Vallée, 5 bd Descartes, 77454 Marne-la-Vallée, France, cyril.roberto@univ-mlv.fr

Benjamin Schlein DPMMS, University of Cambridge, Wilberforce Rd., Cambridge, CB3 0WB, UK

Kareljan Schoutens Institute for Theoretical Physics, University of Amsterdam, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands, kjs@science.uva.nl

Robert Seiringer Departments of Mathematics and Physics, Jadwin Hall, Princeton University, P.O. Box 708, Princeton, NJ 08544, USA, rseiring@princeton.edu

Robert Sims Department of Mathematics, University of Arizona, Tucson, AZ 85721, USA, rsims@math.arizona.edu

Jan Philip Solovej Department of Mathematics, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen, Denmark, solovej@math.ku.dk

Alexander Soshnikov Department of Mathematics, University of California at Davis, One Shields Ave., Davis, CA 95616, USA, soshniko@math.ucdavis.edu

Herbert Spohn Zentrum Mathematik and Physik Department, TU München, Boltzmannstr. 3, 85747 Garching, Germany, spohn@ma.tum.de

Daniel L. Stein Physics Department and Courant Institute of Mathematical Sciences, New York University, New York, NY 10012, USA, daniel.stein@nyu.edu

Sebastian van Strien Mathematics Department, University of Warwick, Coventry CV4 7AL, England, UK, strien@maths.warwick.ac.uk

Toufic M. Suidan Department of Mathematics, The University of Arizona, 617 N. Santa Rita Ave., P.O. Box 210089, Tucson, AZ 85721-0089, USA, tsuidan@math.arizona.edu

Tatiana A. Suslina Faculty of Physics, St. Petersburg State University, Ulyanovskaya, 3, St. Petersburg 198504, Russian Federation, suslina@list.ru

Junji Suzuki Department of Physics, Shizuoka University, Ohya 836, SURUGA, Shizuoka, Japan, sjsuzuk@ipc.shizuoka.ac.jp

Roberto Tateo Dip. di Fisica Teorica and INFN, Università di Torino, Via P. Giuria 1, 10125 Torino, Italy, tateo@to.infn.it

Jörg Teschner DESY Theory, Notkestr. 85, 22603 Hamburg, Germany, teschner@mail.desy.de

Stefan Theisen Max-Planck-Institut für Gravitationsphysik, Albert-Einstein-Institut, Golm, Germany, theisen@aei.mpg.de

Cristina Toninelli LPMA and CNRS UMR 7599, Univ. Paris VI–VII, 4, Pl. Jussieu, 75252 Paris Cedex 05, France, cristina.toninelli@upmc.fr

Craig A. Tracy Department of Mathematics, University of California, Davis, CA 95616, USA, tracy@math.ucdavis.edu

Pierre Vanhove CEA/DSM/SPhT, URA au CNRS, CEA/Saclay, 91191 Gif-sur-Yvette, France, pierre.vanhove@cea.fr

Harold Widom Department of Mathematics, University of California, Santa Cruz, CA 95064, USA, widom@ucsc.edu

Jakob Yngvason Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria; Erwin Schrödinger Institute for Mathematical Physics, Boltzmanngasse 9, 1090 Vienna, Austria, jakob.yngvason@univie.ac.at

Ofer Zeitouni Faculty of Mathematics, Weizmann Institute, Rehovot, Israel; School of Mathematics, University of Minnesota, Minneapolis, USA, zeitouni@math.umn.edu

Contents

Entropy of Eigenfunctions

Nalini Anantharaman, Herbert Koch and Stéphane Nonnenmacher

Abstract We study the high-energy limit for eigenfunctions of the Laplacian, on a compact negatively curved manifold. We review the recent result of Anantharaman–Nonnenmacher (Ann. Inst. Fourier 57(7):2465–2523, 2007) giving a lower bound on the Kolmogorov–Sinai entropy of semiclassical measures. The bound proved here improves that result in the case of variable negative curvature.

1 Motivations

The theory of quantum chaos tries to understand how the chaotic behaviour of a classical Hamiltonian system is reflected in its quantum counterpart. For instance, let M be a compact Riemannian C^∞ manifold, with negative sectional curvatures. The geodesic flow has the Anosov property, which is considered as the ideal chaotic behaviour in the theory of dynamical systems. The corresponding quantum dynamics is the unitary flow generated by the Laplace-Beltrami operator on $L^2(M)$. One expects that the chaotic properties of the geodesic flow influence the spectral theory of the Laplacian. The Random Matrix conjecture [7] asserts that the large eigenvalues should, after proper unfolding, statistically resemble those of a large random matrix, at least for a generic Anosov metric. The Quantum Unique Ergodicity conjecture [26] (see also [6, 30]) describes the corresponding eigenfunctions ψ_k: it claims that the probability measure $|\psi_k(x)|^2 dx$ should approach (in the weak topology) the

Nalini Anantharaman
CMLS, École Polytechnique, 91128 Palaiseau, France, e-mail: nalini@math.polytechnique.fr
Herbert Koch
Mathematical Institute, University of Bonn, Beringstraße 1, 53115 Bonn, Germany, e-mail: koch@math.uni-bonn.de
Stéphane Nonnenmacher
Institut de Physique Théorique, CEA/DSM/PhT, Unité de recherche associée au CNRS, CEA/Saclay, 91191 Gif-sur-Yvette, France, e-mail: snonnenmacher@cea.fr

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Riemannian volume, when the eigenvalue tends to infinity. In fact a stronger property should hold for the *Wigner transform* W_ψ, a function on the cotangent bundle T^*M, (the classical phase space) which simultaneously describes the localization of the wave function ψ in position and momentum.

We will adopt a semiclassical point of view, that is consider the eigenstates of eigenvalue unity of the semiclassical Laplacian $-\hbar^2\triangle$, thereby replacing the high-energy limit by the semiclassical limit $\hbar \to 0$. We denote by $(\psi_k)_{k\in\mathbb{N}}$ an orthonormal basis of $L^2(M)$ made of eigenfunctions of the Laplacian, and by $(-\frac{1}{\hbar_k^2})_{k\in\mathbb{N}}$ the corresponding eigenvalues:

$$-\hbar_k^2\triangle\psi_k = \psi_k, \quad \text{with } \hbar_{k+1} \le \hbar_k. \tag{1}$$

We are interested in the high-energy eigenfunctions of $-\triangle$, in other words the semiclassical limit $\hbar_k \to 0$.

The Wigner distribution associated to an eigenfunction ψ_k is defined by

$$W_k(a) = \langle \mathrm{Op}_{\hbar_k}(a)\psi_k, \psi_k\rangle_{L^2(M)}, \quad a \in C_c^\infty(T^*M).$$

Here $\mathrm{Op}_{\hbar_k}$ is a quantization procedure, set at the scale (wavelength) $\hbar_k$, which associates to any smooth phase space function a (with nice behaviour at infinity) a bounded operator on $L^2(M)$. See for instance [13] or [14] for various quantizations $\mathrm{Op}_\hbar$ on $\mathbb{R}^d$. On a manifold, one can use local coordinates to define Op in a finite system of charts, then glue the objects defined locally thanks to a smooth partition of unity [11]. For standard quantizations $\mathrm{Op}_{\hbar_k}$, the Wigner distribution is of the form $W_k(x,\xi)\,dx\,d\xi$, where $W_k(x,\xi)$ is a smooth function on T^*M, called the Wigner transform of ψ. If a is a function on the manifold M, $\mathrm{Op}_\hbar(a)$ can be taken as the multiplication by a, and thus we have $W_k(a) = \int_M a(x)|\psi_k(x)|^2dx$: the Wigner transform is thus a *microlocal lift* of the density $|\psi_k(x)|^2$. Although the definition of W_k depends on a certain number of choices, like the choice of local coordinates, or of the quantization procedure (Weyl, anti-Wick, "right" or "left" quantization...), its asymptotic behaviour when $\hbar_k \to 0$ does not. Accordingly, we call *semiclassical measures* the limit points of the sequence $(W_k)_{k\in\mathbb{N}}$, in the distribution topology.

In the semiclassical limit, "quantum mechanics converges to classical mechanics". We will denote $|\cdot|_x$ the norm on T_x^*M given by the metric. The geodesic flow $(g^t)_{t\in\mathbb{R}}$ is the Hamiltonian flow on T^*M generated by the Hamiltonian $H(x,\xi) = \frac{|\xi|_x^2}{2}$. A quantization of this Hamiltonian is given by the rescaled Laplacian $-\frac{\hbar^2\triangle}{2}$, which generates the unitary flow $(U_\hbar^t) = (\exp(it\hbar\frac{\triangle}{2}))$ acting on $L^2(M)$. The semiclassical correspondence of the flows $(U_\hbar^t)$ and (g^t) is expressed through the Egorov Theorem:

Theorem 1. *Let $a \in C_c^\infty(T^*M)$. Then, for any given t in $\mathbb{R}$,*

$$\|U_\hbar^{-t}\,\mathrm{Op}_\hbar(a)U_\hbar^t - \mathrm{Op}_\hbar(a\circ g^t)\|_{L^2(M)} = \mathscr{O}(\hbar), \quad \hbar \to 0. \tag{2}$$

The constant implied in the remainder grows (often exponentially) with t, which represents a notorious problem when one wants to study the large time behaviour of

$(U_\hbar^t)$. Typically, the quantum-classical correspondence will break down for times t of the order of the Ehrenfest time (34).

Using (2) and other standard semiclassical arguments, one shows the following:

Proposition 2. *Any semiclassical measure is a probability measure carried on the energy layer $\mathscr{E} = H^{-1}(\frac{1}{2})$ (which coincides with the unit cotangent bundle S^*M). This measure is invariant under the geodesic flow.*

Let us call $\mathfrak{M}$ the set of g^t-invariant probability measures on $\mathscr{E}$. This set is convex and compact for the weak topology. If the geodesic flow has the Anosov property—for instance if M has negative sectional curvature—that set is very large. The geodesic flow has countably many periodic orbits, each of them carrying an invariant probability measure. There are many other invariant measures, like the equilibrium states obtained by variational principles [19], among them the Liouville measure μ_{Liouv}, and the measure of maximal entropy. Note that, for all these examples of measures, the geodesic flow acts ergodically, meaning that these examples are extremal points in $\mathfrak{M}$. Our aim is to determine, at least partially, the set $\mathfrak{M}_{sc}$ formed by all possible semiclassical measures. By its definition, $\mathfrak{M}_{sc}$ is a closed subset of $\mathfrak{M}$, in the weak topology.

For manifolds such that the geodesic flow is ergodic with respect to the Liouville measure, it has been known for some time that *almost all* eigenfunctions become equidistributed over $\mathscr{E}$, in the semiclassical limit. This property is dubbed as Quantum Ergodicity:

Theorem 3 ([27, 32, 11]). *Let M be a compact Riemannian manifold, assume that the action of the geodesic flow on $\mathscr{E} = S^*M$ is ergodic with respect to the Liouville measure. Let $(\psi_k)_{k\in\mathbb{N}}$ be an orthonormal basis of $L^2(M)$ consisting of eigenfunctions of the Laplacian (1), and let (W_k) be the associated Wigner distributions on T^*M.*

Then, there exists a subset $\mathscr{S} \subset \mathbb{N}$ of density 1*, such that*

$$W_k \to \mu_{\text{Liouv}}, \quad k \to \infty,\ k \in \mathscr{S}. \tag{3}$$

The question of existence of "exceptional" subsequences of eigenstates with a different behaviour is still open. On a negatively curved manifold, the geodesic flow satisfies the ergodicity assumption, and in fact much stronger properties: mixing, K-property, etc. For such manifolds, it has been postulated in the Quantum Unique Ergodicity conjecture [26] that the full sequence of eigenstates becomes semiclassically equidistributed over $\mathscr{E}$: one can take $\mathscr{S} = \mathbb{N}$ in the limit (3). In other words, this conjecture states that there exists a unique semiclassical measure, and $\mathfrak{M}_{sc} = \{\mu_{\text{Liouv}}\}$.

So far the most precise results on this question were obtained for manifolds M with constant negative curvature and *arithmetic* properties: see Rudnick–Sarnak [26], Wolpert [31]. In that very particular situation, there exists a countable commutative family of self-adjoint operators commuting with the Laplacian: the Hecke operators. One may thus decide to restrict the attention to common bases of eigen-

functions, often called "arithmetic" eigenstates, or Hecke eigenstates. A few years ago, Lindenstrauss [24] proved that any sequence of arithmetic eigenstates become asymptotically equidistributed. If there is some degeneracy in the spectrum of the Laplacian, note that it could be possible that the Quantum Unique Ergodicity conjectured by Rudnick and Sarnak holds for one orthonormal basis but not for another. On such arithmetic manifolds, it is believed that the spectrum of the Laplacian has bounded multiplicity: if this is really the case, then the semiclassical equidistribution easily extends to any sequence of eigenstates.

Nevertheless, one may be less optimistic when extending the Quantum Unique Ergodicity conjecture to more general systems. One of the simplest example of a symplectic Anosov dynamical system is given by linear hyperbolic automorphisms of the 2-torus, e.g. Arnold's "cat map" $\left(\begin{smallmatrix} 2 & 1 \\ 1 & 1 \end{smallmatrix}\right)$. This system can be quantized into a sequence of $N \times N$ unitary matrices—the propagators, where $N \sim \hbar^{-1}$ [18]. The eigenstates of these matrices satisfy a Quantum Ergodicity theorem similar with Theorem 3, meaning that almost all eigenstates become equidistributed on the torus in the semiclassical limit [9]. Besides, one can choose orthonormal eigenbases of the propagators, such that the whole sequence of eigenstates is semiclassically equidistributed [22]. Still, because the spectra of the propagators are highly degenerate, one can also construct sequences of eigenstates with a different limit measure [16], for instance, a semiclassical measure consisting in two ergodic components: half of it is the Liouville measure, while the other half is a Dirac peak on a single (unstable) periodic orbit. It was also shown that this half-localization is *maximal* for this model [15]: a semiclassical measure cannot have more than half its mass carried by a countable union of periodic orbits. The same type of half-localized eigenstates were constructed by two of the authors for another solvable model, namely the "Walsh quantization" of the baker's map on the torus [3]; for that model, there exist ergodic semiclassical measures of purely fractal type (that is, without any Liouville component). Another type of semiclassical measure was recently obtained by Kelmer for quantized hyperbolic automorphisms on higher-dimensional tori [20]: it consists in the Lebesgue measure on some invariant co-isotropic subspace of the torus.

For these Anosov models on tori, the construction of exceptional eigenstates strongly uses nongeneric algebraic properties of the classical and quantized systems, and cannot be generalized to nonlinear systems.

2 Main Result

In order to understand the set $\mathfrak{M}_{sc}$, we will attempt to compute the *Kolmogorov–Sinai* entropies of semiclassical measures. We work on a compact Riemannian manifold M of arbitrary dimension, and assume that the geodesic flow has the Anosov property. Actually, our method can without doubt be adapted to more general Anosov Hamiltonian systems.

The Kolmogorov–Sinai entropy, also called metric entropy, of a (g^t)-invariant probability measure μ is a nonnegative number $h_{KS}(\mu)$ that describes, in some sense, the complexity of a μ-typical orbit of the flow. The precise definition will be given later, but for the moment let us just give a few facts. A measure carried on a closed geodesic has vanishing entropy. In constant curvature, the entropy is maximal for the Liouville measure. More generally, for any Anosov flow, the energy layer $\mathscr{E}$ is foliated into unstable manifolds of the flow. An upper bound on the entropy of an invariant probability measure is then provided by the Ruelle inequality:

$$h_{KS}(\mu) \leq \left| \int_{\mathscr{E}} \log J^u(\rho) d\mu(\rho) \right|. \tag{4}$$

In this inequality, $J^u(\rho)$ is the *unstable Jacobian* of the flow at the point $\rho \in \mathscr{E}$, defined as the Jacobian of the map g^{-1} restricted to the unstable manifold at the point $g^1\rho$ (note that the average of $\log J^u$ over any invariant measure is negative). The equality holds in (4) if and only if μ is the Liouville measure on $\mathscr{E}$ [23]. If M has dimension d and has constant sectional curvature -1, the above inequality just reads $h_{KS}(\mu) \leq d-1$.

Finally, an important property of the metric entropy is that it is an *affine* functional on $\mathfrak{M}$. According to the Birkhoff ergodic theorem, for any $\mu \in \mathfrak{M}$ and for μ-almost every $\rho \in \mathscr{E}$, the weak limit

$$\mu^\rho = \lim_{|t|\to\infty} \frac{1}{t} \int_0^t \delta_{g^s\rho} ds$$

exists, and is an ergodic probability measure. We can then write

$$\mu = \int_{\mathscr{E}} \mu^\rho d\mu(\rho),$$

which realizes the ergodic decomposition of μ. The affineness of the KS entropy means that

$$h_{KS}(\mu) = \int_{\mathscr{E}} h_{KS}(\mu^\rho) d\mu(\rho).$$

An obvious consequence is the fact that the range of h_{KS} on $\mathfrak{M}$ is an interval $[0, h_{\max}]$.

In the whole article, we consider a certain subsequence of eigenstates $(\psi_{k_j})_{j\in\mathbb{N}}$ of the Laplacian, such that the corresponding sequence of Wigner distributions (W_{k_j}) converges to a semiclassical measure μ. In the following, the subsequence $(\psi_{k_j})_{j\in\mathbb{N}}$ will simply be denoted by $(\psi_\hbar)_{\hbar\to 0}$, using the slightly abusive notation $\psi_\hbar = \psi_{\hbar_{k_j}}$ for the eigenstate ψ_{k_j}. Each eigenstate $\psi_\hbar$ thus satisfies

$$\left(-\hbar^2 \triangle - 1\right)\psi_\hbar = 0. \tag{5}$$

In [2] the first author proved that the entropy of any $\mu \in \mathfrak{M}_{sc}$ is strictly positive. In [4], more explicit lower bounds were obtained. The aim of this paper is to improve the lower bounds of [4] into the following

Theorem 4. *Let μ be a semiclassical measure associated to the eigenfunctions of the Laplacian on M. Then its metric entropy satisfies*

$$h_{KS}(\mu) \geq \left| \int_{\mathscr{E}} \log J^u(\rho) d\mu(\rho) \right| - \frac{(d-1)}{2} \lambda_{\max}, \tag{6}$$

where $d = \dim M$ and $\lambda_{\max} = \lim_{t \to \pm\infty} \frac{1}{t} \log \sup_{\rho \in \mathscr{E}} |dg^t_\rho|$ is the maximal expansion rate of the geodesic flow on $\mathscr{E}$.

In particular, if M has constant sectional curvature -1, we have

$$h_{KS}(\mu) \geq \frac{d-1}{2}. \tag{7}$$

In dimension d, we always have

$$\left| \int_{\mathscr{E}} \log J^u(\rho) d\mu(\rho) \right| \leq (d-1)\lambda_{\max},$$

so the above bound is an improvement over the one obtained in [4],

$$h_{KS}(\mu) \geq \frac{3}{2} \left| \int_{\mathscr{E}} \log J^u(\rho) d\mu(\rho) \right| - (d-1)\lambda_{\max}. \tag{8}$$

In the case of constant or little-varying curvature, the bound (7) is much sharper than the one proved in [2]. On the other hand, if the curvature varies a lot (still being negative everywhere), the right hand side of (6) may actually be negative, in which case the bound is trivial. We believe this "problem" to be a technical shortcoming of our method, and actually conjecture the following bound:

$$h_{KS}(\mu) \geq \frac{1}{2} \left| \int_{\mathscr{E}} \log J^u(\rho) d\mu(\rho) \right|. \tag{9}$$

Extended to the case of the quantized torus automorphisms or the Walsh-quantized baker's map, this bound is saturated for the half-localized semiclassical measures constructed in [16], as well as those obtained in [20, 3]. This bound allows certain ergodic components to be carried by closed geodesics, as long as other components have positive entropy. This may be compared with the following result obtained by Bourgain and Lindenstrauss in the case of arithmetic surfaces:

Theorem 5 ([8]). *Let M be a congruence arithmetic surface, and (ψ_j) an orthonormal basis of eigenfunctions for the Laplacian and the Hecke operators.*

Let μ be a corresponding semiclassical measure, with ergodic decomposition $\mu = \int_{\mathscr{E}} \mu^\rho d\mu(\rho)$. Then, for μ-almost all ergodic components we have $h_{KS}(\mu^\rho) \geq \frac{1}{9}$.

As discussed above, the Liouville measure is the only one satisfying $h_{KS}(\mu) = |\int_{\mathscr{E}} \log J^u(\rho)\, d\mu(\rho)|$ [23], so the Quantum Unique Ergodicity would be proven in one could replace $1/2$ by 1 on the right hand side of (9). However, we believe that (9) is the optimal result that can be obtained without using much more precise information, like for instance a sharp control on the spectral degeneracies, or fine information on the lengths of closed geodesics.

Indeed, in the above mentioned examples of Anosov systems where the Quantum Unique Ergodicity conjecture is wrong and the bound (9) *sharp*, the quantum spectrum has very high degeneracies, which could be responsible for the possibility to construct exceptional eigenstates. Such high degeneracies are not expected in the case of the Laplacian on a negatively curved manifold. For the moment, however, there is no clear understanding of the precise relation between spectral degeneracies and failure of Quantum Unique Ergodicity.

3 Outline of the Proof

We start by recalling the definition and some properties of the metric entropy associated with a probability measure on T^*M, invariant through the geodesic flow. In Sect. 3.2 we extend the notion of entropy to the quantum framework. Our approach is semiclassical, so we want the classical and quantum entropies to be connected in some way when $\hbar \to 0$. The weights appearing in our quantum entropy are estimated in Theorem 6, which was proven and used in [2]. In Sect. 3.2.1 we also compare our quantum entropy with several "quantum dynamical entropies" previously defined in the literature. The proof of Theorem 4 actually starts in Sect. 3.3, where we present the algebraic tool allowing us to take advantage of our estimates (18) (or their optimized version given in Theorem 11), namely an "entropic uncertainty principle" specific of the quantum framework. From Sect. 3.4 on, we apply this "principle" to the quantum entropies appearing in our problem, and proceed to prove Theorem 4. Although the method is basically the same as in [4], several small modifications allow to finally obtain the improved lower bound (6), and also simplify some intermediate proofs, as explained in Remark 12.

3.1 Definition of the Metric Entropy

In this paper we will meet several types of entropies, all of which are defined using the function $\eta(s) = -s \log s$, for $s \in [0, 1]$. We start with the Kolmogorov–Sinai entropy of the geodesic flow with respect to an invariant probability measure.

Let μ be a probability measure on the cotangent bundle T^*M. Let $\mathscr{P} = (E_1, \ldots, E_K)$ be a finite measurable partition of T^*M: $T^*M = \bigsqcup_{i=1}^K E_i$. We will denote the set of indices $\{1, \ldots, K\} = [\![1, K]\!]$. The Shannon entropy of μ with respect to the partition $\mathscr{P}$ is defined as

$$h_{\mathscr{P}}(\mu) = -\sum_{k=1}^{K} \mu(E_k) \log \mu(E_k) = \sum_{k=1}^{K} \eta\big(\mu(E_k)\big).$$

For any integer $n \geq 1$, we denote by $\mathscr{P}^{\vee n}$ the partition formed by the sets

$$E_{\boldsymbol{\alpha}} = E_{\alpha_0} \cap g^{-1} E_{\alpha_1} \cap \cdots \cap g^{-n+1} E_{\alpha_{n-1}}, \tag{10}$$

where $\boldsymbol{\alpha} = (\alpha_0, \ldots, \alpha_{n-1})$ can be any sequence in $[\![1, K]\!]^n$ (such a sequence is said to be of *length* $|\boldsymbol{\alpha}| = n$). The partition $\mathscr{P}^{\vee n}$ is called the n-th refinement of the initial partition $\mathscr{P} = \mathscr{P}^{\vee 1}$. The entropy of μ with respect to $\mathscr{P}^{\vee n}$ is denoted by

$$h_n(\mu, \mathscr{P}) = h_{\mathscr{P}^{\vee n}}(\mu) = \sum_{\boldsymbol{\alpha} \in [\![1,K]\!]^n} \eta\big(\mu(E_{\boldsymbol{\alpha}})\big). \tag{11}$$

If μ is (g^t)-invariant, it follows from the convexity of the logarithm that

$$\forall n, m \geq 1, \quad h_{n+m}(\mu, \mathscr{P}) \leq h_n(\mu, \mathscr{P}) + h_m(\mu, \mathscr{P}), \tag{12}$$

in other words the sequence $(h_n(\mu, \mathscr{P}))_{n \in \mathbb{N}}$ is subadditive. The entropy of μ with respect to the action of the geodesic flow and to the partition $\mathscr{P}$ is defined by

$$h_{KS}(\mu, \mathscr{P}) = \lim_{n \to +\infty} \frac{h_n(\mu, \mathscr{P})}{n} = \inf_{n \in \mathbb{N}} \frac{h_n(\mu, \mathscr{P})}{n}. \tag{13}$$

Each weight $\mu(E_{\boldsymbol{\alpha}})$ measures the μ-probability to visit successively $E_{\alpha_0}, E_{\alpha_1}, \ldots, E_{\alpha_{n-1}}$ at times $0, 1, \ldots, n-1$ through the geodesic flow. Roughly speaking, the entropy measures the exponential decay of these probabilities when n gets large. It is easy to see that $h_{KS}(\mu, \mathscr{P}) \geq \beta$ if there exists C such that $\mu(E_{\boldsymbol{\alpha}}) \leq C\, e^{-\beta n}$, for all n and all $\boldsymbol{\alpha} \in [\![1, K]\!]^n$.

Finally, the Kolmogorov–Sinai entropy of μ with respect to the action of the geodesic flow is defined as

$$h_{KS}(\mu) = \sup_{\mathscr{P}} h_{KS}(\mu, \mathscr{P}), \tag{14}$$

the supremum running over all finite measurable partitions $\mathscr{P}$. The choice to consider the time 1 of the geodesic flow in the definition (10) may seem arbitrary, but the entropy has a natural scaling property: the entropy of μ with respect to the flow (g^{at}) is $|a|$-times its entropy with respect to (g^t).

Assume μ is carried on the energy layer $\mathscr{E}$. Due to the Anosov property of the geodesic flow on $\mathscr{E}$, it is known that the supremum (14) is reached as soon as the diameter of the partition $\mathscr{P} \cap \mathscr{E}$ (that is, the maximum diameter of its elements $E_k \cap \mathscr{E}$) is small enough. Furthermore, let us assume (without loss of generality) that the injectivity radius of M is larger than 1. Then, we may restrict our attention to partitions $\mathscr{P}$ obtained by lifting on $\mathscr{E}$ a partition of the manifold M, that is take $M = \bigsqcup_{k=1}^{K} M_k$ and then $E_k = T^*M_k$. In fact, if the diameter of M_k in M is of order ε, then the diameter of the partition $\mathscr{P}^{\vee 2} \cap \mathscr{E}$ in $\mathscr{E}$ is also of order ε. This

special choice of our partition is not crucial, but it simplifies certain aspects of the analysis.

The existence of the limit in (13), and the fact that it coincides with the infimum, follow from a standard subadditivity argument. It has a crucial consequence: if (μ_i) is a sequence of (g^t)-invariant probability measures on T^*M, weakly converging to a probability μ, and if μ does not charge the boundary of the partition $\mathscr{P}$, we have

$$h_{KS}(\mu, \mathscr{P}) \geq \limsup_i h_{KS}(\mu_i, \mathscr{P}).$$

In particular, assume that for i large enough, the following estimates hold:

$$\forall n \geq 1, \ \forall \boldsymbol{\alpha} \in [\![1, K]\!]^n, \quad \mu_i(E_{\boldsymbol{\alpha}}) \leq C_i \mathrm{e}^{-\beta n}, \tag{15}$$

with β independent of i. This implies for i large enough $h_{KS}(\mu_i, \mathscr{P}) \geq \beta$, and this estimate goes to the limit to yield $h_{KS}(\mu) \geq \beta$.

3.2 From Classical to Quantum Dynamical Entropy

Since our semiclassical measure μ is defined as a limit of Wigner distributions $W_\hbar$, a naive idea would be to estimate from below the KS entropy of $W_\hbar$ and then take the limit $\hbar \to 0$. This idea cannot work directly, because the Wigner transforms $W_\hbar$ are neither positive, nor are they (g^t)-invariant. Therefore, one cannot directly use the (formal) integrals $W_\hbar(E_{\boldsymbol{\alpha}}) = \int_{E_{\boldsymbol{\alpha}}} W_\hbar(x, \xi)\, dx\, d\xi$ to compute the entropy of the semiclassical measure.

Instead, the method initiated by the first author in [2] is based on the following remarks. Each integral $W_\hbar(E_{\boldsymbol{\alpha}})$ can also be written as $W_\hbar(\mathbb{1}_{E_{\boldsymbol{\alpha}}}) = \int_{T^*M} W_\hbar \mathbb{1}_{E_{\boldsymbol{\alpha}}}$, where $\mathbb{1}_{E_{\boldsymbol{\alpha}}}$ is the characteristic function on the set $E_{\boldsymbol{\alpha}}$, that is

$$\mathbb{1}_{E_{\boldsymbol{\alpha}}} = (\mathbb{1}_{E_{\alpha_{n-1}}} \circ g^{n-1}) \times \cdots \times (\mathbb{1}_{E_{\alpha_1}} \circ g) \times \mathbb{1}_{E_{\alpha_0}}. \tag{16}$$

Remember we took $E_k = T^*M_k$, where the M_k form a partition of M.

From the definition of the Wigner distribution, this integral corresponds formally to the overlap $\langle \psi_\hbar, \mathrm{Op}_\hbar(\mathbb{1}_{E_{\boldsymbol{\alpha}}})\psi_\hbar \rangle$. Yet, the characteristic functions $\mathbb{1}_{E_{\boldsymbol{\alpha}}}$ have sharp discontinuities, so their quantizations cannot be incorporated in a nice pseudodifferential calculus. Besides, the set $E_{\boldsymbol{\alpha}}$ is not compactly supported, and shrinks in the unstable direction when $n = |\boldsymbol{\alpha}| \to +\infty$, so that the operator $\mathrm{Op}_\hbar(\mathbb{1}_{E_{\boldsymbol{\alpha}}})$ is very problematic.

We also note that an overlap of the form $\langle \psi_\hbar, \mathrm{Op}_\hbar(\mathbb{1}_{E_{\boldsymbol{\alpha}}})\psi_\hbar \rangle$ is a *hybrid* expression: this is a *quantum* matrix element of an operator defined in terms of the *classical* evolution (16). From the point of view of quantum mechanics, it is more natural to consider, instead, the operator obtained as the product of Heisenberg-evolved quantized functions, namely

$$(U_\hbar^{-n+1} P_{\alpha_{n-1}} U_\hbar^{n-1})(U_\hbar^{-n+2} P_{\alpha_{n-2}} U_\hbar^{n-2}) \cdots (U_\hbar^{-1} P_{\alpha_1} U_\hbar)\, P_{\alpha_0}. \tag{17}$$

Here we used the shorthand notation $P_k = \mathbb{1}_{M_k}$, $k \in [\![1, K]\!]$ (multiplication operators). To remedy the fact that the functions $\mathbb{1}_{M_k}$ are not smooth, which would prevent us from using a semiclassical calculus, we apply a convolution kernel to smooth them, obtain functions $\mathbb{1}^{sm}_{M_k} \in C^\infty(M)$, and consider $P_k \stackrel{\text{def}}{=} \mathbb{1}^{sm}_{M_k}$ (we can do this keeping the property $\sum_{k=1}^K \mathbb{1}^{sm}_{M_k} = 1$).

In the following, we will use the notation $A(t) \stackrel{\text{def}}{=} U_\hbar^{-t} A\, U_\hbar^t$ for the Heisenberg evolution of the operator A though the Schrödinger flow $U_\hbar^t = \exp(-it\hbar\frac{\triangle}{2})$. The norm $\| \bullet \|$ will denote either the Hilbert norm on $L^2(M)$, or the corresponding operator norm. The subsequent "purely quantum" norms were estimated in [2, Theorem 1.3.3]:

Theorem 6 (The main estimate [2]). *Set as above $P_k \stackrel{\text{def}}{=} \mathbb{1}^{sm}_{M_k}$. For every $\mathscr{K} > 0$, there exists $\hbar_{\mathscr{K}} > 0$ such that, uniformly for all $\hbar < \hbar_{\mathscr{K}}$, for all $n \leq \mathscr{K}|\log\hbar|$, for all $(\alpha_0, \dots, \alpha_{n-1}) \in [\![1, K]\!]^n$,*

$$\| P_{\alpha_{n-1}}(n-1)\, P_{\alpha_{n-2}}(n-2) \cdots P_{\alpha_0}\, \psi_\hbar \| \leq 2(2\pi\hbar)^{-d/2}\, \mathrm{e}^{-\frac{\Lambda}{2}n}(1 + \mathscr{O}(\varepsilon))^n. \quad (18)$$

The exponent Λ is given by the "smallest expansion rate":

$$\Lambda = -\sup_{\nu\in\mathfrak{M}} \int \log J^u(\rho) d\nu(\rho) = \inf_\gamma \sum_{i=1}^{d-1} \lambda_i^+(\gamma).$$

The infimum on the right hand side runs over the set of closed orbits on $\mathscr{E}$, and the λ_i^+ denote the positive Lyapunov exponents along the orbit, that is the logarithms of the expanding eigenvalues of the Poincaré map, divided by the period of the orbit. The parameter $\varepsilon > 0$ is an upper bound on the diameters of the supports of the functions $\mathbb{1}^{sm}_{M_k}$ in M.

From now on we will call the product operator

$$P_{\boldsymbol{\alpha}} = P_{\alpha_{n-1}}(n-1)\, P_{\alpha_{n-2}}(n-2) \cdots P_{\alpha_0}, \quad \boldsymbol{\alpha} \in [\![1, K]\!]^n. \quad (19)$$

To prove the above estimate, one actually controls the operator norm

$$\| P_{\boldsymbol{\alpha}}\, \mathrm{Op}_\hbar(\chi) \| \leq 2(2\pi\hbar)^{-d/2}\, \mathrm{e}^{-\frac{\Lambda}{2}n}(1 + \mathscr{O}(\varepsilon))^n, \quad (20)$$

where $\chi \in C_c^\infty(\mathscr{E}^\varepsilon)$ is an energy cutoff such that $\chi = 1$ near $\mathscr{E}$, supported inside a neighbourhood $\mathscr{E}^\varepsilon = H^{-1}([\frac{1}{2} - \varepsilon, \frac{1}{2} + \varepsilon])$ of $\mathscr{E}$.

In quantum mechanics, the matrix element $\langle \psi_\hbar, P_{\boldsymbol{\alpha}}\psi_\hbar \rangle$ looks like the "probability", for a particle in the state $\psi_\hbar$, to visit successively the phase space regions $E_{\alpha_0}, E_{\alpha_1}, \dots, E_{\alpha_{n-1}}$ at times $0, 1, \dots, n-1$ of the Schrödinger flow. Theorem 6 implies that this "probability" decays exponentially fast with n, with rate $\frac{\Lambda}{2}$, but this decay only starts around the time

$$n_1 \stackrel{\text{def}}{=} \frac{d|\log\hbar|}{\Lambda}, \quad (21)$$

which is a kind of "Ehrenfest time" (see (34) for another definition of Ehrenfest time).

Yet, because the matrix elements $\langle \psi_\hbar, P_{\boldsymbol{\alpha}} \psi_\hbar \rangle$ are not real in general, they can hardly be used to define a "quantum measure". Another possibility to define the probability for the particle to visit the sets E_{α_k} at times k, is to take the squares of the norms appearing in (18):

$$\| P_{\boldsymbol{\alpha}}\, \psi_\hbar \|^2 = \| P_{\alpha_{n-1}}(n-1)\, P_{\alpha_{n-2}}(n-2) \cdots P_{\alpha_0} \psi_\hbar \|^2. \tag{22}$$

Now we require the smoothed characteristic functions $\mathbb{1}_{M_i}^{sm}$ to satisfy the identity

$$\sum_{k=1}^{K} \left(\mathbb{1}_{M_k}^{sm}(x) \right)^2 = 1 \quad \text{for any point } x \in M. \tag{23}$$

We denote by $\mathscr{P}_{sm}$ the smooth partition of M made by the functions $((\mathbb{1}_{M_k}^{sm})^2)_{k=1}^K$. The corresponding set of multiplication operators $(P_k)_{k=1}^K \stackrel{\text{def}}{=} \mathscr{P}_q$ forms a "quantum partition of unity":

$$\sum_{k=1}^{K} P_k^2 = Id_{L^2}. \tag{24}$$

For any $n \geq 1$, we refine the quantum partition $\mathscr{P}_q$ into $(P_{\boldsymbol{\alpha}})_{|\boldsymbol{\alpha}|}$, as in (19). The weights (22) exactly add up to unity, so it makes sense to consider the entropy

$$h_n(\psi_\hbar, \mathscr{P}_q) \stackrel{\text{def}}{=} \sum_{\boldsymbol{\alpha} \in [\![1, K]\!]^n} \eta\big(\| P_{\boldsymbol{\alpha}}\, \psi_\hbar \|^2 \big). \tag{25}$$

3.2.1 Connection with Other Quantum Entropies

This entropy appears to be a particular case of the "general quantum entropies" described by Słomczyński and Życzkowski [29], who already had in mind applications to quantum chaos. In their terminology, a family of bounded operators $\pi = (\pi_k)_{k=1}^{\mathscr{N}}$ on a Hilbert space $\mathscr{H}$ satisfying

$$\sum_{k=1}^{\mathscr{N}} \pi_k^*\, \pi_k = Id_{\mathscr{H}} \tag{26}$$

provides an "instrument" which, to each index $k \in [\![1, \mathscr{N}]\!]$, associates the following map on density matrices:

$$\rho \mapsto \mathscr{I}(k)\rho = \pi_k\, \rho\, \pi_k^*, \quad \text{a nonnegative operator with } \operatorname{tr}(\mathscr{I}(k)\rho) \leq 1.$$

From a unitary propagator U and its adjoint action $\mathscr{U}\rho = U\rho U^{-1}$, they propose to construct the refined instrument

$$\mathscr{I}(\boldsymbol{\alpha})\rho \stackrel{\text{def}}{=} \mathscr{I}(\alpha_{n-1}) \circ \cdots \circ \mathscr{U} \circ \mathscr{I}(\alpha_1) \circ \mathscr{U} \circ \mathscr{I}(\alpha_0)\rho = U^{-n+1}\, \pi_{\boldsymbol{\alpha}}\, \rho\, \pi_{\boldsymbol{\alpha}}^*\, U^{n-1},$$
$$\boldsymbol{\alpha} \in [\![1, \mathscr{N}]\!]^n,$$

where we used (19) to refine the operators π_k into $\pi_{\boldsymbol{\alpha}}$. We obtain the probability weights

$$\mathrm{tr}(\mathscr{I}(\boldsymbol{\alpha})\rho) = \mathrm{tr}(\pi_{\boldsymbol{\alpha}}\rho\pi_{\boldsymbol{\alpha}}^*), \quad \boldsymbol{\alpha} \in [\![1, \mathscr{N}]\!]^n. \tag{27}$$

For any U-invariant density ρ, these weights provide an entropy

$$h_n(\rho, \mathscr{I}) = \sum_{\boldsymbol{\alpha}\in[\![1,\mathscr{N}]\!]^n} \eta\big(\mathrm{tr}(\mathscr{I}(\boldsymbol{\alpha})\rho)\big). \tag{28}$$

One easily checks that our quantum partition $\mathscr{P}_q = (P_k)_{k=1}^K$ satisfies (26), and that if one takes $\rho = |\psi_\hbar\rangle\langle\psi_\hbar|$ the weights $\mathrm{tr}(\mathscr{I}(\boldsymbol{\alpha})\rho)$ exactly correspond to our weights $\|P_{\boldsymbol{\alpha}}\psi\|^2$. Hence, the entropy (28) coincides with (25).

Around the same time, Alicki and Fannes [1] used the same quantum partition (26) (which they called "finite operational partitions of unity") to define a different type of entropy, now called the "Alicki–Fannes entropy" (the definition extends to general C^*-dynamical systems). For each $n \geq 1$ they extend the weights (27) to "off-diagonal entries" to form a $\mathscr{N}^n \times \mathscr{N}^n$ density matrix ρ_n:

$$[\rho_n]_{\boldsymbol{\alpha}',\boldsymbol{\alpha}} = \mathrm{tr}(\pi_{\boldsymbol{\alpha}'}\, \rho\, \pi_{\boldsymbol{\alpha}}^*), \quad \boldsymbol{\alpha}, \boldsymbol{\alpha}' \in [\![1, \mathscr{N}]\!]^n. \tag{29}$$

The AF entropy of the system $(\mathscr{U}, \rho)$ is then defined as follows: take the Von Neumann entropy of these density matrices, $h_n^{AF}(\rho, \pi) = \mathrm{tr}\ \eta(\rho_n)$, then take $\limsup_{n\to\infty} \frac{1}{n} h_n^{AF}(\rho, \pi)$ and finally take the supremum over all possible finite operational partitions of unity π.

We mention that traces of the form (29) also appear in the "quantum histories" approach to quantum mechanics (see e.g. [17], and [29, Appendix D] for references).

3.2.2 Naive Treatment of the Entropy $h_n(\psi_\hbar, \mathscr{P}_q)$

For fixed $|\boldsymbol{\alpha}| > 0$, the Egorov theorem shows that $\|P_{\boldsymbol{\alpha}}\psi_\hbar\|^2$ converges to the classical weight $\mu((\mathbb{1}_{M_{\boldsymbol{\alpha}}}^{sm})^2)$ when $\hbar \to 0$, so for fixed $n > 0$ the entropy $h_n(\psi_\hbar, \mathscr{P}_q)$ converges to $h_n(\mu, \mathscr{P}_{sm})$, defined as in (11), the characteristic functions $\mathbb{1}_{M_k}$ being replaced by their smoothed versions $(\mathbb{1}_{M_k}^{sm})^2$. On the other hand, from the estimate (20) the entropies $h_n(\psi_\hbar, \mathscr{P}_q)$ satisfy, for $\hbar$ small enough,

$$h_n(\psi_\hbar, \mathscr{P}_q) \geq n\big(\Lambda + \mathscr{O}(\varepsilon)\big) - d|\log\hbar| + \mathscr{O}(1), \tag{30}$$

for any time $n \leq \mathscr{K}|\log\hbar|$. For large times $n \approx \mathscr{K}|\log\hbar|$, this provides a lower bound

$$\frac{1}{n} h_n(\psi_\hbar, \mathscr{P}_q) \geq \big(\Lambda + \mathscr{O}(\varepsilon)\big) - \frac{d}{\mathscr{K}} + \mathscr{O}(1/|\log\hbar|),$$

which looks very promising since $\mathscr{K}$ can be taken arbitrary large: we could be tempted to take the semiclassical limit, and deduce a lower bound $h_{KS}(\mu) \geq \Lambda$.

Unfortunately, this does not work, because in the range $\{n > n_1\}$ where the estimate (30) is useful, the Egorov theorem breaks down, the weights (22) do not approximate the classical weights $\mu((\mathbb{1}^{sm}_{M_\alpha})^2)$, and there is no relationship between $h_n(\psi, \mathscr{P}_q)$ and the classical entropies $h_n(\mu, \mathscr{P}_{sm})$.

This breakdown of the quantum-classical correspondence around the Ehrenfest time is ubiquitous for chaotic dynamics. It has been observed before when studying the connection between the Alicki–Fannes entropy for the quantized torus automorphisms and the KS entropy of the classical dynamics [5]: the quantum entropies $h_n^{AF}(\psi_\hbar, \mathscr{P}_q)$ follow the classical $h_n(\mu, \mathscr{P}_{sm})$ until the Ehrenfest time (and therefore grow linearly with n), after which they "saturate", to produce a vanishing entropy $\limsup_{n\to\infty} \frac{1}{n} h_n^{AF}(\psi_\hbar, \mathscr{P}_q)$.

To prove Theorem 4, we will still use the estimates (20), but in a more subtle way, namely by referring to an *entropic uncertainty principle*.

3.3 Entropic Uncertainty Principle

The theorem below is an adaptation of the entropic uncertainty principle conjectured by Deutsch and Kraus [12, 21] and proved by Massen and Uffink [25]. These authors were investigating the theory of measurement in quantum mechanics. Roughly speaking, this result states that if a unitary matrix has "small" entries, then any of its eigenvectors must have a "large" Shannon entropy.

Let $(\mathscr{H}, \langle ., . \rangle)$ be a complex Hilbert space, and denote $\|\psi\| = \sqrt{\langle \psi, \psi \rangle}$ the associated norm. Consider a quantum partition of unity $(\pi_k)_{k=1}^{\mathscr{N}}$ on $\mathscr{H}$ as in (26). If $\|\psi\| = 1$, we define the entropy of ψ with respect to the partition π as in (25), namely $h_\pi(\psi) = \sum_{k=1}^{\mathscr{N}} \eta(\|\pi_k \psi\|^2)$. We extend this definition by introducing the notion of *pressure*, associated to a family $\boldsymbol{v} = (v_k)_{k=1,\dots,\mathscr{N}}$ of positive real numbers: the pressure is defined by

$$p_{\pi,\boldsymbol{v}}(\psi) \stackrel{\text{def}}{=} \sum_{k=1}^{\mathscr{N}} \eta\big(\|\pi_k \psi\|^2\big) - \sum_{k=1}^{\mathscr{N}} \|\pi_k \psi\|^2 \log v_k^2.$$

In Theorem 7, we actually need two partitions of unity $(\pi_k)_{k=1}^{\mathscr{N}}$ and $(\tau_j)_{j=1}^{\mathscr{M}}$, and two families of weights $\boldsymbol{v} = (v_k)_{k=1}^{\mathscr{N}}$, $\boldsymbol{w} = (w_j)_{j=1}^{\mathscr{M}}$, and consider the corresponding pressures $p_{\pi,\boldsymbol{v}}(\psi)$, $p_{\tau,\boldsymbol{w}}(\psi)$. Besides the appearance of the weights $\boldsymbol{v}$, $\boldsymbol{w}$, we bring another modification to the statement in [25] by introducing an auxiliary operator $\mathscr{O}$.

Theorem 7 ([4, Theorem 6.5]). *Let $\mathscr{O}$ be a bounded operator and $\mathscr{U}$ be an isometry on $\mathscr{H}$.*

Define $c_{\mathscr{O}}^{(\boldsymbol{v},\boldsymbol{w})}(\mathscr{U}) \stackrel{\text{def}}{=} \sup_{j,k} w_j v_k \|\tau_j \mathscr{U} \pi_k^* \mathscr{O}\|$, and $V = \max_k v_k$, $W = \max_j w_j$. Then, for any $\epsilon \geq 0$, for any normalized $\psi \in \mathscr{H}$ satisfying

$$\forall k = 1, \dots, \mathscr{N}, \quad \|(Id - \mathscr{O})\,\pi_k\,\psi\| \leq \epsilon, \tag{31}$$

the pressures $p_{\tau,\boldsymbol{w}}(\mathscr{U}\,\psi)$, $p_{\pi,\boldsymbol{v}}(\psi)$ *satisfy*

$$p_{\tau,\boldsymbol{w}}(\mathscr{U}\,\psi) + p_{\pi,\boldsymbol{v}}(\psi) \geq -2\log\left(c_{\mathscr{O}}^{(\boldsymbol{v},\boldsymbol{w})}(\mathscr{U}) + \mathscr{N}\,V\,W\,\epsilon\right).$$

Example 8. The original result of [25] corresponds to the case where $\mathscr{H} = \mathbb{C}^{\mathscr{N}}$, $\mathscr{O} = Id$, $\epsilon = 0$, $\mathscr{N} = \mathscr{M}$, $v_k = w_j = 1$, and the operators $\pi_k = \tau_k$ are the orthogonal projectors on some orthonormal basis $(e_k)_{k=1}^{\mathscr{N}}$ of $\mathscr{H}$. In this case, the theorem asserts that

$$h_\pi(\mathscr{U}\,\psi) + h_\pi(\psi) \geq -2\log c(\mathscr{U})$$

where $c(\mathscr{U}) = \sup_{j,k} |\langle e_k, \mathscr{U} e_j\rangle|$ is the supremum of all matrix elements of $\mathscr{U}$ in the orthonormal basis (e_k). As a special case, one gets $h_\pi(\psi) \geq -\log c(\mathscr{U})$ if ψ is an eigenfunction of $\mathscr{U}$.

3.4 Applying the Entropic Uncertainty Principle to the Laplacian Eigenstates

In this section we explain how to use Theorem 7 in order to obtain nontrivial information on the quantum entropies (25) and then $h_{KS}(\mu)$. For this we need to define the data to input in the theorem. Except the Hilbert space $\mathscr{H} = L^2(M)$, all other data depend on the semiclassical parameter $\hbar$: the quantum partition π, the operator $\mathscr{O}$, the positive real number ϵ, the weights (v_j), (w_k) and the unitary operator $\mathscr{U}$.

As explained in Sect. 3.2, we partition M into $M = \bigsqcup_{k=1}^{K} M_k$, consider open sets $\Omega_k \ni M_k$ (which we assume to have diameters $\leq \varepsilon$), and consider smoothed characteristic functions $\mathbb{1}_{M_k}^{sm}$ supported respectively inside Ω_k, and satisfying the identity (23). The associated multiplication operators on $\mathscr{H}$ are form a quantum partition $(P_k)_{k=1}^{K}$, which we had called $\mathscr{P}_q$. To alleviate notations, we will drop the subscript q.

From (24), and using the unitarity of $U_\hbar$, one realizes that for any $n \geq 1$, the families of operators $\mathscr{P}^{\vee n} = (P_{\boldsymbol{\alpha}}^*)_{|\boldsymbol{\alpha}|=n}$ and $\mathscr{T}^{\vee n} = (P_{\boldsymbol{\alpha}})_{|\boldsymbol{\alpha}|=n}$ (see (19)) make up two quantum partitions of unity as in (26), of cardinal K^n.

3.4.1 Sharp Energy Localization

In the estimate (20), we introduced an energy cutoff χ on a finite energy strip $\mathscr{E}^\varepsilon$, with $\chi \equiv 1$ near $\mathscr{E}$. This cutoff does not appear in the estimate (18), because, when applied to the eigenstate $\psi_\hbar$, the operator $\mathrm{Op}_\hbar(\chi)$ essentially acts like the identity.

The estimate (20) will actually not suffice to prove Theorem 4. We will need to optimize it by replacing χ in (20) with a "sharp" energy cutoff. For some fixed

(small) $\delta \in (0,1)$, we consider a smooth function $\chi_\delta \in C^\infty(\mathbb{R};[0,1])$, with $\chi_\delta(t) = 1$ for $|t| \leq \mathrm{e}^{-\delta/2}$ and $\chi_\delta(t) = 0$ for $|t| \geq 1$. Then, we rescale that function to obtain the following family of $\hbar$-dependent cutoffs near $\mathscr{E}$:

$$\begin{aligned} &\forall \hbar \in (0,1),\ \forall n \in \mathbb{N},\ \forall \rho \in T^*M, \\ &\chi^{(n)}(\rho;\hbar) \stackrel{\text{def}}{=} \chi_\delta\big(\mathrm{e}^{-n\delta}\,\hbar^{-1+\delta}(H(\rho)-1/2)\big). \end{aligned} \tag{32}$$

The cutoff $\chi^{(n)}$ is supported in a tubular neighbourhood of $\mathscr{E}$ of width $2\hbar^{1-\delta}\,\mathrm{e}^{n\delta}$. We will always assume that this width is $\ll \hbar^{1/2}$ in the semiclassical limit, which is the case if we ensure that $n \leq C_\delta |\log\hbar|$ for some $0 < C_\delta < (2\delta)^{-1} - 1$. In spite of their singular behaviour, these cutoffs can be quantized into pseudodifferential operators $\mathrm{Op}(\chi^{(n)})$ described in [4] (the quantization uses a pseudodifferential calculus adapted to the energy layer $\mathscr{E}$, drawn from [28]). The eigenstate $\psi_\hbar$ is indeed very localized near $\mathscr{E}$, since it satisfies

$$\big\|\big(\mathrm{Op}(\chi^{(0)}) - 1\big)\psi_\hbar\big\| = \mathscr{O}(\hbar^\infty)\|\psi_\hbar\|. \tag{33}$$

In the rest of the paper, we also fix a small $\delta' > 0$, and call "Ehrenfest time" the $\hbar$-dependent integer

$$n_E(\hbar) \stackrel{\text{def}}{=} \left\lfloor \frac{(1-\delta')|\log\hbar|}{\lambda_{\max}} \right\rfloor. \tag{34}$$

Notice the resemblance with the time n_1 defined in (21). The significance of this time scale will be discussed in Sect. 3.4.5.

The following proposition states that the operators $(P^*_{\boldsymbol{\alpha}})_{|\boldsymbol{\alpha}|=n_E}$, almost preserve the energy localization of $\psi_\hbar$:

Proposition 9. *For any $L > 0$, there exists $\hbar_L$ such that, for any $\hbar \leq \hbar_L$, the Laplacian eigenstate satisfies*

$$\forall \boldsymbol{\alpha},\ |\boldsymbol{\alpha}| = n_E, \quad \big\|\big(\mathrm{Op}(\chi^{(n_E)}) - Id\big)P^*_{\boldsymbol{\alpha}}\,\psi_\hbar\big\| \leq \hbar^L\|\psi_\hbar\|. \tag{35}$$

We recognize here a condition of the form (31).

3.4.2 Applying Theorem 7: Step 1

We now precise some of the data we will use in the entropic uncertainty principle, Theorem 7. As opposed to the choice made in [4], we will use two different partitions π, τ.

- The quantum partitions π and τ are given respectively by the families of operators $\pi = \mathscr{P}^{\vee n_E} = (P^*_{\boldsymbol{\alpha}})_{|\boldsymbol{\alpha}|=n_E}$, $\tau = \mathscr{T}^{\vee n_E} = (P_{\boldsymbol{\alpha}})_{|\boldsymbol{\alpha}|=n_E}$. Notice that these partitions only differ by the ordering of the operators $P_{\alpha_i}(i)$ inside the products. In the semiclassical limit, these partitions have cardinality $\mathscr{N} = K^{n_E} \asymp \hbar^{-K_0}$ for some fixed $K_0 > 0$.
- The isometry will be the propagator at the Ehrenfest time, $\mathscr{U} = U_\hbar^{n_E}$.

- The auxiliary operator is given as $\mathscr{O} = \mathrm{Op}(\chi^{(n_E)})$, and the error $\epsilon = \hbar^L$, where L will be chosen very large (see Sect. 3.4.4).
- The weights $v_{\boldsymbol{\alpha}}$, $w_{\boldsymbol{\alpha}}$ will be selected in Sect. 3.4.4. They will be semiclassically tempered, meaning that there exists $K_1 > 0$ such that, for $\hbar$ small enough, all $v_{\boldsymbol{\alpha}}$, $w_{\boldsymbol{\alpha}}$ are contained in the interval $[1, \hbar^{-K_1}]$.

The entropy and pressures associated with a state $\psi \in \mathscr{H}$ are given by

$$h_\pi(\psi) = \sum_{|\boldsymbol{\alpha}|=n_E} \eta\big(\|P_{\boldsymbol{\alpha}}^*\,\psi\|^2\big), \tag{36}$$

$$p_{\pi,\boldsymbol{v}}(\psi) = h_\pi(\psi) - 2\sum_{|\boldsymbol{\alpha}|=n_E} \|P_{\boldsymbol{\alpha}}^*\,\psi\|^2 \log v_{\boldsymbol{\alpha}}. \tag{37}$$

With respect to the second partition, we have

$$h_\tau(\psi) = \sum_{|\boldsymbol{\alpha}|=n_E} \eta\big(\|P_{\boldsymbol{\alpha}}\,\psi\|^2\big), \tag{38}$$

$$p_{\tau,\boldsymbol{w}}(\psi) = h_\tau(\psi) - 2\sum_{|\boldsymbol{\alpha}|=n_E} \|P_{\boldsymbol{\alpha}}\,\psi\|^2 \log w_{\boldsymbol{\alpha}}. \tag{39}$$

We notice that the entropy $h_\tau(\psi)$ exactly corresponds to the formula (25), while $h_\pi(\psi)$ is built from the norms

$$\|P_{\boldsymbol{\alpha}}^*\,\psi\|^2 = \|P_{\alpha_0} P_{\alpha_1}(1)\cdots P_{\alpha_{n-1}}(n-1)\,\psi\|^2.$$

If ψ is an eigenfunction of $U_\hbar$, the above norm can be obtained from (22) by exchanging $U_\hbar$ with $U_\hbar^{-1}$, and replacing the sequence $\boldsymbol{\alpha} = (\alpha_0, \ldots, \alpha_{n-1})$ by $\bar{\boldsymbol{\alpha}} \overset{\text{def}}{=} (\alpha_{n-1}, \ldots, \alpha_0)$. So the entropies $h_\pi(\psi)$ and $h_\tau(\psi)$ are mapped to one another through the time reversal $U_\hbar \to U_\hbar^{-1}$.

With these data, we draw from Theorem 7 the following

Corollary 10. *For $\hbar > 0$ small enough consider the data π, τ, $\mathscr{U}$, $\mathscr{O}$ as defined above. Let*

$$c_{\mathscr{O}}^{\boldsymbol{v},\boldsymbol{w}}(\mathscr{U}) \overset{\text{def}}{=} \max_{|\boldsymbol{\alpha}|=|\boldsymbol{\alpha}'|=n_E} \big(w_{\boldsymbol{\alpha}'}\, v_{\boldsymbol{\alpha}}\, \|P_{\boldsymbol{\alpha}'}\, U_\hbar^{n_E}\, P_{\boldsymbol{\alpha}}\, \mathrm{Op}(\chi^{(n_E)})\|\big). \tag{40}$$

Then for any normalized state ϕ satisfying (35),

$$p_{\tau,\boldsymbol{w}}(U_\hbar^{n_E}\,\phi) + p_{\pi,\boldsymbol{v}}(\phi) \geq -2\log\left(c_{\mathscr{O}}^{\boldsymbol{v},\boldsymbol{w}}(\mathscr{U}) + h^{L-K_0-2K_1}\right).$$

From (35), we see that the above corollary applies to the eigenstate $\psi_\hbar$ if $\hbar$ is small enough.

The reason to take the same value n_E for the refined partitions $\mathscr{P}^{\vee n_E}$, $\mathscr{T}^{\vee n_E}$ and the propagator $U_\hbar^{n_E}$ is the following: the products appearing in $c_{\mathscr{O}}^{\boldsymbol{v},\boldsymbol{w}}(\mathscr{U})$ can be rewritten (with $U \equiv U_\hbar$):

$$P_{\boldsymbol{\alpha}'}\, U^{n_E}\, P_{\boldsymbol{\alpha}} = U^{-n_E+1} P_{\alpha'_{n_E-1}} U \cdots U P_{\alpha'_0} U P_{\alpha_{n_E-1}} U \cdots U P_{\alpha_0} = U^{n_E}\, P_{\boldsymbol{\alpha}\boldsymbol{\alpha}'}.$$

Thus, the estimate (20) with $n = 2n_E$ already provides an upper bound for the norms appearing in (40)—the replacement of χ by the sharp cutoff $\chi^{(n_E)}$ does not harm the estimate.

To prove Theorem 4, we actually need to improve the estimate (20), as was done in [4], see Theorem 11 below. This improvement is done at two levels: we will use the fact that the cutoffs $\chi^{(n_E)}$ are sharper than χ, and also the fact that the expansion rate of the geodesic flow (which governs the upper bound in (20)) is not uniform, but depends on the sequence $\boldsymbol{\alpha}$.

Our choice for the weights $v_{\boldsymbol{\alpha}}$, $w_{\boldsymbol{\alpha}}$ will then be guided by the $\boldsymbol{\alpha}$-dependent upper bounds given in Theorem 11. To state that theorem, we introduce some notations.

3.4.3 Coarse-Grained Unstable Jacobian

We recall that, for any energy $\lambda > 0$, the geodesic flow g^t on the energy layer $\mathscr{E}(\lambda) = H^{-1}(\lambda) \subset T^*M$ is Anosov, so that the tangent space $T_\rho \mathscr{E}(\lambda)$ at each $\rho \in T^*M$, $H(\rho) > 0$ splits into

$$T_\rho \mathscr{E}(\lambda) = E^u(\rho) \oplus E^s(\rho) \oplus \mathbb{R}\, X_H(\rho)$$

where E^u (resp. E^s) is the unstable (resp. stable) subspace. The unstable Jacobian $J^u(\rho)$ is defined by $J^u(\rho) = \det(dg^{-1}_{|E^u(g^1\rho)})$ (the unstable spaces at ρ and $g^1\rho$ are equipped with the induced Riemannian metric).

This Jacobian can be "discretized" as follows in the energy strip $\mathscr{E}^\varepsilon \supset \mathscr{E}$. For any pair of indices $(\alpha_0, \alpha_1) \in [\![1, K]\!]^2$, we define

$$J_1^u(\alpha_0, \alpha_1) \stackrel{\text{def}}{=} \sup\{J^u(\rho) : \rho \in T^*\Omega_{\alpha_0} \cap \mathscr{E}^\varepsilon,\ g^1\rho \in T^*\Omega_{\alpha_1}\} \tag{41}$$

if the set on the right hand side is not empty, and $J_1^u(\alpha_0, \alpha_1) = e^{-R}$ otherwise, where $R > 0$ is a fixed large number. For any sequence of symbols $\boldsymbol{\alpha}$ of length n, we define

$$J_n^u(\boldsymbol{\alpha}) \stackrel{\text{def}}{=} J_1^u(\alpha_0, \alpha_1) \cdots J_1^u(\alpha_{n-2}, \alpha_{n-1}). \tag{42}$$

Although J^u and $J_1^u(\alpha_0, \alpha_1)$ are not necessarily everywhere smaller than unity, there exists $C, \lambda_+, \lambda_- > 0$ such that, for any $n > 0$, for any $\boldsymbol{\alpha}$ with $|\boldsymbol{\alpha}| = n$,

$$C^{-1}\, \mathrm{e}^{-n(d-1)\,\lambda_+} \le J_n^u(\boldsymbol{\alpha}) \le C\, \mathrm{e}^{-n(d-1)\,\lambda_-}. \tag{43}$$

One can take $\lambda_+ = \lambda_{\max}(1 + \varepsilon)$, where $\lambda_{\max}$ is the maximal expanding rate in Theorem 4. We now give our central estimate, easy to draw from [4, Corollary 3.4].

Theorem 11. *Fix small positive constants $\varepsilon, \delta, \delta'$ and a constant $0 < C_\delta < (2\delta)^{-1} - 1$. Take an open cover $M = \bigcup_k \Omega_k$ of diameter $\le \varepsilon$ and an associated quantum partition $\mathscr{P} = (P_k)_{k=1}^K$. There exists $\hbar_0$ such that, for any $\hbar \le \hbar_0$, for any positive integer $n \le C_\delta |\log \hbar|$, and any pair of sequences $\boldsymbol{\alpha}$, $\boldsymbol{\alpha}'$ of length n,*

$$\left\| P_{\boldsymbol{\alpha}\boldsymbol{\alpha}'} \operatorname{Op}(\chi^{(n)}) \right\| = \left\| P_{\boldsymbol{\alpha}'} U_\hbar^n P_{\boldsymbol{\alpha}} \operatorname{Op}(\chi^{(n)}) \right\| \leq C \hbar^{-\frac{d-1}{2}-\delta} \mathrm{e}^{n\delta} \sqrt{J_n^u(\boldsymbol{\alpha}) J_n^u(\boldsymbol{\alpha}')}. \tag{44}$$

The constant C only depends on the Riemannian manifold (M, g). If we take $n = n_E$, this takes the form

$$\| P_{\boldsymbol{\alpha}'} U_\hbar^{n_E} P_{\boldsymbol{\alpha}} \operatorname{Op}(\chi^{(n_E)}) \| \leq C \hbar^{-\frac{d-1+c\delta}{2}} \sqrt{J_{n_E}^u(\boldsymbol{\alpha}) J_{n_E}^u(\boldsymbol{\alpha}')}, \tag{45}$$

where $c = 2 + 2\lambda_{\max}^{-1}$.

The idea of proof in Theorem 11 is rather simple, although the technical implementation is cumbersome. We first show that for any normalized state ψ, the state $\operatorname{Op}(\chi^{(n)})\psi$ can be essentially decomposed into a superposition of $\hbar^{-d}|\operatorname{supp}\chi^{(n)}|$ normalized Lagrangian states, supported on Lagrangian manifolds transverse to the stable foliation. In fact the Lagrangian states we work with are truncated δ-functions, supported on Lagrangians of the form $\bigcup_t g^t S_z^* M$. The action of the operator $U^n P_{\boldsymbol{\alpha}\boldsymbol{\alpha}'} = P_{\alpha'_{n-1}} U \cdots U P_{\alpha_0}$ on such Lagrangian states can be analyzed through WKB methods, and is simple to understand at the classical level: each application of the propagator U stretches the Lagrangian along the unstable direction (the rate of stretching being described by the local unstable Jacobian), whereas each operator P_k "projects" on a piece of Lagrangian of diameter ε. This iteration of stretching and cutting accounts for the exponential decay. The $\boldsymbol{\alpha}\boldsymbol{\alpha}'$-independent factor on the right of (45) results from adding together the contributions of all the initial Lagrangian states. Notice that this prefactor is smaller than in Theorem 6 due to the condition $C_\delta < (2\delta)^{-1} - 1$.

Remark 12. In [4] we used the same quantum partition $\mathscr{P}^{\vee n_E}$ for π and τ in Theorem 7. As a result, we needed to estimate from above the norms $\| P_{\boldsymbol{\alpha}'}^* U^{n_E} P_{\boldsymbol{\alpha}} \times \operatorname{Op}(\chi^{(n_E)}) \|$ (see [4, Theorem. 2.6]). The proof of this estimate was much more involved than the one for (45), since it required to control long pieces of unstable manifolds. By using instead the two partitions $\mathscr{P}^{(n)}$, $\mathscr{T}^{(n)}$, we not only prove a more precise lower bound (6) on the KS entropy, but also short-circuit some fine dynamical analysis.

3.4.4 Applying Theorem 7: Step 2

There remains to choose the weights $(v_{\boldsymbol{\alpha}}, w_{\boldsymbol{\alpha}})$ to use in Theorem 7. Our choice is guided by the following idea: in (40), the weights should balance the variations (with respect to $\boldsymbol{\alpha}, \boldsymbol{\alpha}'$) in the norms, such as to make all terms in (40) of the same order. Using the upper bounds (45), we end up with the following choice for all $\boldsymbol{\alpha}$ of length n_E:

$$v_{\boldsymbol{\alpha}} = w_{\boldsymbol{\alpha}} \stackrel{\text{def}}{=} J_{n_E}^u(\boldsymbol{\alpha})^{-1/2}.$$

From (43), there exists $K_1 > 0$ such that, for $\hbar$ small enough, all the weights are contained in the interval $[1, \hbar^{-K_1}]$, as announced in Sect. 3.4.2. Using these weights, the estimate (45) implies the following bound on the coefficient (40):

$$\forall \hbar < \hbar_0, \quad c_{\mathscr{O}}^{\boldsymbol{v},\boldsymbol{w}}(\mathscr{U}) \leq C\, \hbar^{-\frac{d-1+c\delta}{2}}.$$

We can now apply Corollary 10 to the particular case of the eigenstates $\psi_\hbar$. We choose L such that $L - K_0 - 2K_1 > -\frac{d-1+c\delta}{2}$, so from Corollary 10 we draw the following

Proposition 13. *Let $(\psi_\hbar)_{\hbar\to 0}$ be our sequence of eigenstates (5). In the semiclassical limit, the pressures of $\psi_\hbar$ satisfy*

$$p_{\mathscr{P}^{\vee n_E},\boldsymbol{v}}(\psi_\hbar) + p_{\mathscr{T}^{\vee n_E},\boldsymbol{w}}(\psi_\hbar) \geq -\frac{(d-1+c\delta)\lambda_{\max}}{(1-\delta')}\, n_E + \mathscr{O}(1). \tag{46}$$

If M has constant curvature we have $\log J_{\boldsymbol{\alpha}}^n \leq -n(d-1)\lambda_{\max}(1-\mathscr{O}(\varepsilon))$ for all $\boldsymbol{\alpha}$ of length n, and the above lower bound can be written

$$h_{\mathscr{P}^{\vee n_E}}(\psi_\hbar) + h_{\mathscr{T}^{\vee n_E}}(\psi_\hbar) \geq (d-1)\lambda_{\max}\big(1+\mathscr{O}(\varepsilon,\delta,\delta')\big)\, n_E.$$

As opposed to (30), the above inequality provides a nontrivial lower bound for the quantum entropies at the time n_E, which is smaller than the time n_1 of (21), and will allow to connect those entropies to the KS entropy of the semiclassical measure (see below).

3.4.5 Subadditivity Until the Ehrenfest Time

Even at the relatively small time n_E, the connection between the quantum entropy $h(\psi_\hbar, \mathscr{P}^{\vee n_E})$ and the classical $h(\mu, \mathscr{P}_{sm}^{\vee n_E})$ is not completely obvious: both are sums of a large number of terms ($\asymp \hbar^{-K_0}$). Before taking the limit $\hbar \to 0$, we will prove that a lower bound of the form (46) still holds if we replace $n_E \asymp |\log\hbar|$ by some fixed $n_o \in \mathbb{N}$, and $\mathscr{P}^{\vee n_E}$ by the corresponding quantum partition $\mathscr{P}^{\vee n_o}$. The link between quantum pressures at times n_E and n_o is provided by the following *subadditivity property*, which is the semiclassical analogue of the classical subadditivity of pressures for invariant measures (see (12)).

Proposition 14 (Subadditivity). *Let $\delta' > 0$. There is a function $R(n_o,\hbar)$, and a real number $R > 0$ independent of δ', such that, for any integer $n_o \geq 1$,*

$$\limsup_{\hbar\to 0} |R(n_o,\hbar)| \leq R$$

and with the following properties. For any small enough $\hbar > 0$, any integers n_o, $n \in \mathbb{N}$ with $n_o + n \leq n_E(\hbar)$, for any $\psi_\hbar$ normalized eigenstate satisfying (5), the following inequality holds:

$$p_{\mathscr{P}^{\vee(n_o+n)},\boldsymbol{v}}(\psi_\hbar) \leq p_{\mathscr{P}^{\vee n_o},\boldsymbol{v}}(\psi_\hbar) + p_{\mathscr{P}^{\vee n},\boldsymbol{v}}(\psi_\hbar) + R(n_o,\hbar).$$

The same inequality is satisfied by the pressures $p_{\mathscr{T}^{\vee n},\boldsymbol{w}}(\psi_\hbar)$.

To prove this proposition, one uses a refined version of Egorov's theorem [10] to show that the non-commutative dynamical system formed by $(U_\hbar^t)$ acting (through Heisenberg) on observables supported near $\mathscr{E}$ is (approximately) commutative on time intervals of length $n_E(\hbar)$. Precisely, we showed in [4] that, provided ε is small enough, for any $a, b \in C_c^\infty(\mathscr{E}^\varepsilon)$,

$$\forall t \in [-n_E(\hbar), n_E(\hbar)], \quad \big\|[\mathrm{Op}_\hbar(a)(t), \mathrm{Op}_\hbar(b)]\big\| = \mathscr{O}(\hbar^{c\delta'}), \quad \hbar \to 0,$$

and the implied constant is uniform with respect to t. Within that time interval, the operators $P_{\alpha_j}(j)$ appearing in the definition of the pressures commute up to small semiclassical errors. This almost commutativity explains why the quantum pressures $p_{\mathscr{P}^{\vee n}, \boldsymbol{v}}(\psi_\hbar)$ satisfy the same subadditivity property as the classical entropy (12), for times smaller than n_E.

Thanks to this subadditivity, we may finish the proof of Theorem 4. Fixing n_o, using for each $\hbar$ the Euclidean division $n_E(\hbar) = q(\hbar)\, n_o + r(\hbar)$ (with $r(\hbar) < n_o$), Proposition 14 implies that for $\hbar$ small enough,

$$\frac{p_{\mathscr{P}^{\vee n_E}, \boldsymbol{v}}(\psi_\hbar)}{n_E} \le \frac{p_{\mathscr{P}^{\vee n_o}, \boldsymbol{v}}(\psi_\hbar)}{n_o} + \frac{p_{\mathscr{P}^{\vee r}, \boldsymbol{v}}(\psi_\hbar)}{n_E} + \frac{R(n_o, \hbar)}{n_o}.$$

The same inequality is satisfied by the pressures $p_{\mathscr{T}^{\vee n}, \boldsymbol{w}}(\psi_\hbar)$. Using (46) and the fact that $p_{\mathscr{P}^{\vee r}, \boldsymbol{v}}(\psi_\hbar)$ stays uniformly bounded when $\hbar \to 0$, we find

$$\begin{aligned}\frac{p_{\mathscr{P}^{\vee n_o}, \boldsymbol{v}}(\psi_\hbar) + p_{\mathscr{T}^{\vee n_o}, \boldsymbol{w}}(\psi_\hbar)}{n_o} \ge & -\frac{2(d-1+c\delta)\lambda_{\max}}{2(1-\delta')} - \frac{2R(n_o, \hbar)}{n_o} \\ & + \mathscr{O}_{n_o}(1/n_E). \end{aligned} \tag{47}$$

We are now dealing with quantum partitions $\mathscr{P}^{\vee n_o}$, $\mathscr{T}^{\vee n_o}$, for $n_0 \in \mathbb{N}$ independent of $\hbar$. At this level the quantum and classical entropies are related through the (finite time) Egorov theorem, as we had noticed in Sect. 3.2.2. For any $\boldsymbol{\alpha}$ of length n_o, the weights $\|P_{\boldsymbol{\alpha}}\, \psi_\hbar\|^2$ and $\|P_{\boldsymbol{\alpha}}^*\, \psi_\hbar\|^2$ both converge to $\mu((\mathbb{1}_{M_{\boldsymbol{\alpha}}}^{sm})^2)$, where we recall that

$$\mathbb{1}_{M_{\boldsymbol{\alpha}}}^{sm} = (\mathbb{1}_{M_{\alpha_{n_o-1}}}^{sm} \circ g^{n_o-1}) \times \cdots \times (\mathbb{1}_{M_{\alpha_1}}^{sm} \circ g) \times \mathbb{1}_{M_{\alpha_0}}^{sm}.$$

Thus, both entropies $h_{\mathscr{P}^{\vee n_o}}(\psi_\hbar)$, $h_{\mathscr{T}^{\vee n_o}}(\psi_\hbar)$ semiclassically converge to the classical entropy $h_{n_o}(\mu, \mathscr{P}_{sm})$. As a result, the left hand side of (47) converges to

$$2\,\frac{h_{n_o}(\mu, \mathscr{P}_{sm})}{n_o} + \frac{2}{n_o} \sum_{|\boldsymbol{\alpha}|=n_o} \mu\big((\mathbb{1}_{M_{\boldsymbol{\alpha}}}^{sm})^2\big)\, \log J_{n_o}^u(\boldsymbol{\alpha}). \tag{48}$$

Since μ is g^t-invariant and $J_{n_o}^u$ has the multiplicative structure (42), the second term in (48) can be simplified:

$$\sum_{|\boldsymbol{\alpha}|=n_o} \mu\big((\mathbb{1}_{M_{\boldsymbol{\alpha}}}^{sm})^2\big)\, \log J_{n_o}^u(\boldsymbol{\alpha}) = (n_o - 1) \sum_{\alpha_0, \alpha_1} \mu\big((\mathbb{1}_{M_{(\alpha_0,\alpha_1)}}^{sm})^2\big)\, \log J_1^u(\alpha_0, \alpha_1).$$

We have thus obtained the lower bound

$$\frac{h_{n_o}(\mu, \mathscr{P}_{sm})}{n_o} \geq -\frac{n_o - 1}{n_o} \sum_{\alpha_0, \alpha_1} \mu\big((\mathbb{1}^{sm}_{M_{(\alpha_0,\alpha_1)}})^2\big) \log J^{\mu}_1(\alpha_0, \alpha_1) - \frac{(d - 1 + c\delta)\lambda_{\max}}{2(1 - \delta')} - \frac{R}{n_o}. \tag{49}$$

At this stage we may forget about δ and δ'. The above lower bound does not depend on the derivatives of the functions $\mathbb{1}^{sm}_{M_\alpha}$, so the same bound carries over if we replace $\mathbb{1}^{sm}_{M_\alpha}$ by the characteristic functions $\mathbb{1}_{M_\alpha}$. We can finally let n_o tend to $+\infty$, then let the diameter ε tend to 0. The left hand side converges to $h_{KS}(\mu)$ while, from the definition (41), the sum in the right hand side of (49) converges to the integral $\int_{\mathscr{E}} \log J^u(\rho) d\mu(\rho)$ as $\varepsilon \to 0$, which proves (6).

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Stability of Doubly Warped Product Spacetimes

Lars Andersson *

Abstract Nonlinear stability for a class of doubly warped spacetimes is proved. The background spacetimes have negative Einstein factors. It shown that for dimension $D \geq 11$ there is a full parameter family of solutions to the vacuum Einstein equations which has Kasner-like singularity and Friedmann like asympotics in the future. In particular, these spacetimes have crushing singularity and are globally foliated by constant mean curvature Cauchy hypersurfaces.

1 Introduction

The goal of this paper is to prove the existence of a full parameter family of future complete spacetimes with quiescent singularity. In the paper [1], written jointly with Mark Heinzle, we studied a class of generalized Kasner spacetimes. These are $D = m + n + 1$ dimensional Lorentzian doubly warped product spacetimes of the form $\mathbb{R} \times M \times N$ with line element

$$-dt^2 + a^2(t)g + b^2(t)h,$$

where (M, g) and (N, h) are m- and n-dimensional Einstein spaces. We shall here consider only the case where M, N are negative Einstein spaces.

The paper [1] showed that the spacetimes under consideration have a Kasner-like singularity, while the future asympotics is Friedmann-like. In that paper it was demonstrated that for dimension $D \geq 10$, a Kaluza-Klein dimensional reduction gives a spacetime with eternal acceleration. Further, and most importantly for the

Lars Andersson
Department of Mathematics, University of Miami, Coral Gables, FL 33124, USA and Albert Einstein Institute, Am Mühlenberg 1, 14476 Golm, Germany, e-mail: larsa@math.miami.edu

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application in the present paper, it was demonstrated in [1] that the singularity allows AVTD deformations exactly when $D \geq 11$. This is the case we consider here.

In a recent paper of the author with Vincent Moncrief [4], we proved the nonlinear stability to the future for a class of Lorentz cone spacetimes. The background spaces considered are Lorentz cones over negative Einstein spaces. The work in [4] allows general dimension and further allows the Riemannian Einstein factor to have a non-trivial Einstein moduli space. A $3+1$ dimensional case of this situation was considered in [4], there rigidity was assumed. This condition has later been removed in the $3+1$ dimensional case by Martin Reiris [10].

In the present paper, we apply the results of [3] as well as the analysis in [1], together with the Fuchsian techniques developed with Alan Rendall in [5], see also [7] for the higher dimensional case, to demonstrate for $D \geq 11$, the existence of a full parameter family of nonlinearly stable deformations of the generalized Kasner spacetimes studied in [1]. These deformations have dynamics and geometry which is controlled globally *from the singularity to the infinite future*. In particular, they have crushing singularity, admit a global foliation by CMC Cauchy hypersurfaces, and are future causally geodesically complete. This is the first result of its type.

2 Warped Product Spacetimes

Let (M, γ^M), (N, γ^N) be m- and n-dimensional compact negative Einstein spaces with

$$\mathrm{Ric}_{\gamma^M} = -(m+n-1)\gamma^M, \qquad \mathrm{Ric}_{\gamma^N} = -(m+n-1)\gamma^N.$$

We consider line elements on a $D = m+n+1$ dimensional spacetime $\mathbb{R} \times M \times N$ of the form

$$-dt^2 + a^2(t)\gamma^M + b^2(t)\gamma^N. \tag{1}$$

The vacuum Einstein equations for the line elements of the form (1) were analyzed in [1] in terms of scale invariant variables. Let

$$p = -\frac{\dot{a}}{a}, \qquad q = -\frac{\dot{b}}{b}.$$

The mean curvature τ is given by

$$\tau = mp + nq.$$

The scale invariant variables are[2]

$$P = \frac{p}{\tau}, \qquad Q = \frac{q}{\tau}, \qquad A = -\frac{1}{a\tau}, \qquad B = -\frac{1}{b\tau}.$$

[2] In [1], mean curvature is denoted by H and the time variable τ used there is related to the proper time by $\partial_\tau = H^{-1}\partial_t$. With this definition, T/τ is a negative constant. Here, we use notation adapted to [2].

Here A, B may be viewed as curvature variables. Define the scale invariant time coordinate T by

$$\partial_T = -\tau^{-1}\partial_t = -\tau\partial_\tau.$$

The Einstein equations in terms of the time T for P, Q, A, B forms an autonomous system, and the evolution equation for τ decouples.

The phase space of the scale invariant system resulting from the Einstein equations for the line element (1), with M, N negative Einstein spaces, is a topologically a disc. There are five equilibrium points, four of which (F_1), (F_2) and (F_A), (F_B) are on the boundary, where $AB = 0$, and one (F_*) is in the interior, where $AB > 0$. See Fig. 1 for a schematic of the phase portrait for the case $D \geq 11$, in which case (F_*) is a stable node. In this note, we shall be interested only in this case.

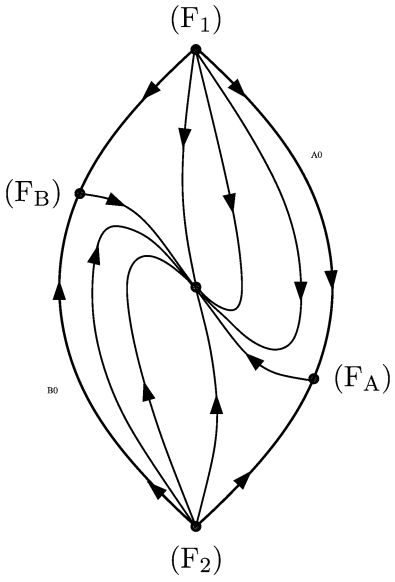

Fig. 1 Phase portrait for $D \geq 11$, see [1]

The equilibrium points on the boundary correspond to cosmological singularities with asymptotically Kasner-like behavior. Generic past directed orbits tend to one of the two equilibrium points ($F_{1,2}$) which are characterized by the relations

$$A = B = 0, \qquad mP^2 + nQ^2 = 1, \qquad mP + nQ = 1,$$

All future directed orbits tend to the equilibrium point (F_*), characterized by

$$A = B = P = Q = \frac{1}{m+n}$$

with asymptotically Friedmann-like behavior. In particular the spacetime geometry is asymptotic in the expanding direction to the Lorentz cone

$$-dt^2 + \frac{t^2}{(m+n)^2}\gamma, \tag{2}$$

where

$$\gamma = (m+n)^2\big(\gamma^M + \gamma^N\big) \tag{3}$$

is an Einstein metric with constant $-(m+n-1)/(m+n)^2$ on $M \times N$. The t-level sets are constant mean curvature hypersurfaces, and as we shall see the warped product spacetimes under consideration are, up to a time reparametrization, in CMCSH gauge with respect to γ.

2.1 Asymptotic Behavior

By the results of [1, Sect. 3.4], a, b have, in the case of spacetime dimension $D \geq 11$, the following asymptotic form in the expanding direction, i.e. at (F_*), as $t \nearrow \infty$,

$$a = t\big[1 + nc_0 t^{-\lambda^*} + O(t^{-2\lambda^*})\big], \tag{4a}$$

$$b = t\big[1 - mc_0 t^{-\lambda^*} + O(t^{-2\lambda^*})\big] \tag{4b}$$

cf. [1, (3.8)], as $t \to \infty$, where $\lambda^* > 0$ is given by

$$\lambda^* = \frac{1}{2}(m+n-1-\sqrt{(m+n-1)(m+n-9)}).$$

The induced metric on the Cauchy surface $M \times N$ at time t is given by

$$a^2(t)\gamma_M + b^2(t)\gamma_N. \tag{5}$$

The Christoffel symbol of this metric contains no mixed terms, and due to the scale invariance of the Christoffel symbol it is identical to the Christoffel symbol of the metric (3). It follows that the tension field defined with respect to the metric (5) and γ vanishes and hence (1) is automatically in CMCSH gauge with respect to the background metric γ. The second fundamental form is

$$pa^2\gamma^M_{ij} + qb^2\gamma^N_{ij} \tag{6}$$

and from (4), we have

$$\tau = -(m+n)t^{-1} + O(t^{-1-2\lambda^*}).$$

Recall from [4, Sect. 4] that the scale invariant Cauchy data (g, Σ) are related to the metric and second fundamental form by

$$g_{ij} = \tau^2 \tilde{g}_{ij}, \quad \Sigma_{ij} = \tau\left(\tilde{K}_{ij} - \frac{\tau}{n+m}\tilde{g}_{ij}\right).$$

Let $(\hat{g}, \hat{\Sigma})$ be the scale invariant data corresponding to the metric (5) and the second fundamental form (6). A calculation using (4) gives

$$\hat{\Sigma} = t^{-\lambda^*}(1-\lambda^*)c_0\left[n\gamma^M - m\gamma^N\right] + O(t^{-2\lambda^*}), \tag{7a}$$

$$\hat{g} - \gamma = t^{-\lambda^*}(m+n)^2 c_0\left[n\gamma^M - m\gamma^N\right] + O(t^{-2\lambda^*}). \tag{7b}$$

The scale invariant time is $T = -\log(-\tau/(m+n))$. Due to the fact that there are no spatial degrees of freedom in $(\hat{g}, \hat{\Sigma})$, the asymptotic form the Cauchy data given in (7) immediately allows us to estimate the Sobolev distance of the scale invariant data $(\hat{g}, \hat{\Sigma})$ from the background data $(\gamma, 0)$. We have for any $s \geq 1$,

$$\|\hat{g} - \gamma\|_{H^s} + \|\hat{\Sigma}\|_{H^{s-1}} = O(e^{-\lambda^* T}) \tag{8}$$

or equivalently

$$\|\hat{g} - \gamma\|_{H^s} + \|\hat{K} + \gamma\|_{H^{s-1}} = O(e^{-\lambda^* T}),$$

where $\hat{K} = \tau\tilde{K}$ is the scale invariant second fundamental form. Similarly, inserting the calculated form of $\hat{\Sigma}$, $\hat{g} - \gamma$ into the energies E_s, we have for $s \geq 1$,

$$E_s = O(e^{-2\lambda^* T}),$$

which tends to zero as $T \to \infty$.

Next we consider the asymptotic behavior of a generic orbit in the collapsing direction, asymptotic to one of the equilibrium points (F_1), (F_2). A generic solution is of the form

$$a = a_0 t^P\left[1 + O(t^\delta)\right], \qquad b = b_0 t^Q\left[1 + O(t^\delta)\right] \tag{9}$$

for constants a_0, b_0, P, Q, and for some $\delta > 0$. Here P, Q are solutions to

$$mP + nQ = 1, \qquad mP^2 + nQ^2 = 1. \tag{10}$$

It follows from these equations that $|P| < 1$, $|Q| < 1$.

3 Fuchsian Method

The generalized Kasner exponents can be defined as the eigenvalues of the scale-invariant second fundamental form $K_i{}^j$, with one index raised using the scale invariant spatial metric g_{ij}. By [1, Theorem 3.1] and [1, Proposition 3.2], $t = 0$ corresponds to a cosmological singularity, in the sense that $a(t), b(t) \to 0$, as $t \to 0$ so that the induced metric on the t-level sets collapses. Further, the singularity at $t = 0$ is Kasner like, i.e. the generalized Kasner exponents converge as $t \to 0$.

The Fuchsian method allows one to construct families of solutions to the Einstein equations, with controlled behavior at a cosmological singularity, under condition that the behavior at the singularity is asymptotically velocity dominated. This means roughly that asymptotically at the singularity, spatial derivatives become insignificant and the dynamics of the Einstein equations approaches that of a family of Bianchi I spacetimes, one for each spatial point. This method was first applied to Gowdy models by Kichenassamy and Rendall [9]. The first treatment of case of the Einstein equations without symmetry was given by Andersson and Rendall [5], for the $3+1$ dimensional Einstein equations minimally coupled with a massless scalar field. The application of the Fuchsian method to the vacuum Einstein equations in $D = d + 1$ spacetime dimensions was carried out by Damour, Henneaux, Rendall and Weaver [7].

The Fuchsian method applies a singular version of the Cauchy-Kowalevski theorem, and therefore requires the velocity dominated data to be real analytic in the spatial direction. Although real analytic functions are dense in C^∞ in a compact manifold this is an important restriction, and it is desirable to generalize the results discussed here to cover smooth data or data with finite regularity. In particular it is important to prove a stability type result that shows that there is an open set of initial data, in Sobolev norm, which leads to spacetimes with asymptotically velocity dominated behavior. This was shown by Ringstrom for the Gowdy case, see [11].

The main result of the Fuchsian analysis in the case we are interested in, is that given a velocity dominated solution which satisfies certain restrictions, see below, there is a unique solution to the vacuum Einstein equations, which has the same asymptotic generalized Kasner exponents at each point as those of the velocity dominated solution. Further, the solution produced by the Fuchsian method is asymptotic to the velocity dominated solution at the singularity.

Let $p_1 \leq p_2 \leq \cdots \leq p_d$ be limiting Kasner exponents as $t \to 0$, in increasing order. By [1, Sect. 4], for $D \geq 11$, the generic spacetime of the form (1) has generalized Kasner exponents whose limit at the singularity satisfy

$$1 + p_1 - p_d - p_{d-1} > 0. \tag{11}$$

This is precisely those doubly warped product spacetimes which are past asymptotic to one of the equilibrium points ($\mathrm{F}_{1,2}$). According to the results of [7], see in particular [7, Sect. 3], this implies that one may apply the Fuchsian method to construct a full parameter family of non-homogeneous spacetimes deforming the warped product ones.

3.1 Velocity Dominated Equations

In order to construct the approximating spacetime, we must specify a "velocity dominated" seed solution. This is defined from initial data $({}^0g_{ij}, {}^0K_i{}^j)$ which satisfy the velocity dominated constraint equations [5], see [7, Sect. 2.3] for the case of space-

times of general dimension. These are in the vacuum case,

$$-{}^0K_i{}^j{}^0K^j{}_i + (\mathrm{tr}\,{}^0K)^2 = 0, \tag{12}$$

$${}^0\tilde{\nabla}_j{}^0K^j{}_i - {}^0\tilde{\nabla}_i(\mathrm{tr}\,{}^0K) = 0 \tag{13}$$

a truncated form of the Einstein vacuum constraints. By a modification of the conformal method, one may construct a full parameter family of solutions to the velocity dominated constraints.

The velocity dominated solution is constructed by solving the velocity dominated evolution equations

$$\partial_t{}^0g_{ij} = -2{}^0K_{ij}, \tag{14a}$$

$$\partial_t{}^0K^i{}_j = (\mathrm{tr}\,{}^0K){}^0K^i{}_j. \tag{14b}$$

Again, this system is a truncated form of the full Einstein evolution equations. Equations (14) has, up to time-reparametrization, solutions of the form

$${}^0K^a{}_b(t) = -t^{-1}\kappa^a{}_b, \tag{15}$$

$${}^0g_{ab}(t) = {}^0g_{ac}(t_0)\big[(t/t_0)^{2\kappa}\big]^c{}_b, \tag{16}$$

$\mathrm{tr}\,\kappa = 1$. For each spatial point, the equations are just the equations modelling a Bianchi I, or Kasner spacetime.

3.2 Velocity Dominated Solution

The velocity dominated solution which correspond to the warped product spacetimes with the Kasner-like behavior at the singularity given by (9) has spatial metric

$${}^0\hat{g} = a_0^2t^{2P}\gamma^M + b_0^2t^{2Q}\gamma^N, \tag{17a}$$

and the covariant second fundamental form is

$${}^0\hat{K} = -t^{-1}\big(Pa_0^2t^{2P}\gamma^M + Qb_0^2t^{2P}\gamma^N\big). \tag{17b}$$

There is a unique spacetime asymptotic to the velocity dominated solution at the singularity, provided (11) holds. By [1, Sect. 4] this condition is satisfied for the warped product spacetimes of the form (1), asymptotic in the past to one of the equilibrium points ($\mathrm{F}_{1,2}$), if $D \geq 11$. The solution to the Einstein equations corresponding to the velocity dominated data (17) is, by uniqueness, the warped product spacetime with this asymptotic behavior. This is a one-parameter family of spacetimes, up to a trivial rescaling.

Fix a_0, b_0 and let $(\hat{g}, \hat{K})$ be the scale-invariant data for the warped product metric with velocity dominated data given by (17). The map from the velocity dominated data $({}^0g(t_0), {}^0K(t_0))$ to the data $(\tilde{g}, \tilde{K})$ at t_0 for the vacuum spacetime constructed by the Fuchsian method with seed solution $({}^0g, {}^0K)$ is continuous at the background data velocity dominated data $({}^0\hat{g}, {}^0\hat{K})$, in terms of the natural topology on the space of real analytic tensors on M. See [5, 7] for details, and in particular [6] for analytical details concerning the singular form of the Cauchy-Kowalewski theorem.

The construction gives a full parameter set of real analytic spacetimes close to the background spacetime. The topology on the space of analytic functions is finer than the H^s Sobolev topology for any s. Hence, the scale invariant data (g, Σ) are H^s close to $(\hat{g}, \hat{\Sigma})$. We summarize this discussion in the following lemma.

Lemma 1. *Fix $t_0 > 0$. For each $s \geq 1$, $\epsilon > 0$, there is a full parameter set of velocity dominated data $({}^0g(t_0), {}^0K(t_0))$ close to the background velocity dominated data of the form (17), such that*

$$\|g(t_0) - \hat{g}(t_0)\|_s + \|K(t_0) - \hat{K}(t_0)\|_{s-1} < \epsilon,$$

where (g, K) are scale invariant data for the vacuum spacetime with velocity dominated data $({}^0g, {}^0K)$ and $(\hat{g}, \hat{K})$ are the scale invariant data corresponding to the warped product background metric with velocity dominated data given by (17).

4 Stability

The spacetime with rescaled data $(\tilde{g}, \tilde{K})$ given by Lemma 1 is not CMC foliated in the time coordinate t. We will now show that the spacetimes can be refoliated in CMC time, with the small data condition still valid.

Lemma 2. *Assume the Einstein spaces M, N are stable, with smooth deformation spaces. Fix $\tau_0 < 0$. For each $s \geq 1$, $\epsilon > 0$, there is a $t_0 > 0$ and a full parameter set of velocity dominated data $({}^0g(t_0), {}^0K(t_0))$ close to the background velocity dominated data of the form (17), such that the spacetime produced by the Fuchsian method from the velocity dominate data contains a CMC foliation with mean curvature τ taking values in an interval containing $(-\infty, \tau_0)$, and such that at mean curvature time τ_0 we have*

$$\|g(\tau_0) - \hat{g}(\tau_0)\|_s + \|K(\tau_0) - \hat{K}(\tau_0)\|_{s-1} < \epsilon, \tag{18}$$

where (g, K) are scale invariant data for the vacuum spacetime with velocity dominated data $({}^0g, {}^0K)$ and $(\hat{g}, \hat{K})$ are the scale invariant data corresponding to the warped product background metric with velocity dominated data given by (17). Further, (g, K) are satisfy the CMCSH gauge condition and the shadow metric condition with respect to the background metric γ on $M \times N$.

Proof. The spacetime produced by the Fuchsian method is asymptotically Kasner-like at the singularity, and in particular the singularity is crushing. Recall that the

time t_0 in Lemma 1 is arbitrary. The mean curvature for the warped product background metric takes all values in $(-\infty, 0)$ and for velocity dominated data sufficiently close to the background data, we have by a suitable choice of t_0 in Lemma 1, $\mathrm{tr}_{\tilde{g}} \tilde{K}(t_0) > \tau_0$. This means that the Cauchy surface at time t_0 is a barrier for the mean curvature equation, and hence by [8], there is a CMC foliation with mean curvature taking values in an interval containing $(-\infty, \tau_0)$. Due to the elliptic nature of the CMC equation, the smallness condition (18) is satisfied for velocity dominated data sufficiently close to the background.

By assumption the Einstein spaces M, N are stable, with smooth deformation space. By [4, Sect. 3] that this is true also for $(M \times N, \gamma)$. By the work in [4, Sect. 4.2], we may after possibly decreasing ϵ and acting on the background warped product metric with a time-independent diffeomorphism, assume that the data produced above satisfies the CMCSH gauge and the shadow-metric condition with respect to an Einstein metric $\bar{\gamma}$ close to γ and in the deformation space $\mathcal{V}$ of γ. Due to the local uniformization result [4, Proposition 2.4] $\bar{\gamma}$ is of the form (3) with respect to two Einstein metrics $\bar{\gamma}^M, \bar{\gamma}^N$ close to γ^M, γ^N. The Einstein equations for the warped product spacetimes are independent of the choice of Einstein metric. Hence this modified background has the same dynamics as the original one and we may without loss of generality assume the CMCSH and shadow metric condition is satisfied with respect to the original background data. This completes the proof of the lemma. □

We are now ready to apply the above construction of a CMC foliated, quiescent spacetime, together with the main result of [4], to prove the existence of a full parameter family of quiescent, future complete spacetimes. In Sect. 2.1 we proved that the data $(\hat{g}, \hat{\Sigma})$ corresponding to the warped product background spacetime tends, in Sobolev norm, to the data corresponding to the Lorentz cone metric (2). Together with the smallness estimate in Lemma 2 this means that by suitable choosing τ_0, ϵ, the data for the quiescent spacetime constructed by the Fuchsian method satisfies, at CMC time τ_0, the conditions of the stability theorem [4, Theorem 7.1]. This gives

Theorem 3. *Assume M, N are stable with smooth deformation space. Further, assume $D \geq 11$. Then, there is a full parameter set of velocity dominated data $({}^0g, {}^0K)$ close to the velocity dominated data $({}^0\hat{g}, {}^0\hat{K})$, corresponding to a warped product spacetime of the form (1), with a Kasner-like initial singularity with generalized Kasner exponents close to P, Q satisfying equation (10), such that the quiescent spacetime constructed using the Fuchsian method admits a global CMC foliation, and is asymptotic to the Lorentz cone spacetime with line element (2).*

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Rigorous Construction of Luttinger Liquids Through Ward Identities

Giuseppe Benfatto

Abstract There are up to now two different ways to prove the key property on which our Luttinger liquid rigorous construction rests, the vanishing of the leading part of the Beta function. The first one was developed in the last years and is based in an essential way on the exact Mattis-Lieb solution of the Luttinger model. More recently, we found a new proof, based on the Ward identities obtained by a chiral local gauge transformation, applied to a Luttinger model with ultraviolet and infrared cutoffs. This is an old approach in the physical literature, but its implementation in an RG scheme is not trivial at all, because the ultraviolet and infrared cutoffs destroy local gauge invariance and produce "correction terms" with respect to the formal Ward identities. We discover however a new set of identities, called "Correction Identities", relating the corrections to the Schwinger functions. By combining Ward and Correction identities with a Dyson equation, the vanishing of the Beta function follows, so that the infrared cutoff can be removed. As a byproduct, even the ultraviolet cutoff can be removed, after a suitable ultraviolet renormalization, so that a Quantum Field Theory corresponding to the Thirring model is constructed, showing the phenomenon of Chiral anomaly.

1 Introduction

There are many fermion models (one-dimensional Fermi gas at low temperature [1], XYZ model [2], a large class of classical two-dimensional spin systems, like Ashkin-Teller model [6]), whose rigorous infrared RG analysis is based on two key properties:

(1) The flow of the effective coupling (the beta function) is the same, up to exponentially small terms, as the analogous flow for the spinless Tomonaga model

Giuseppe Benfatto
Dipartimento di Matematica, Università di Roma "Tor Vergata", Via della Ricerca Scientifica, 00133 Rome, Italy, e-mail: benfatto@mat.uniroma2.it

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(that is the Luttinger model with ultraviolet cutoff and local interaction, which is equivalent to the Thirring model with fixed ultraviolet cutoff).

(2) The beta function for this special model (which is not solvable) is asymptotically vanishing, so that the effective coupling on large scales is essentially constant and of the same order of the coupling on small scales.

Up to now there are two different ways to prove property (2). The first one was developed in the last years and is based in an essential way on the exact Mattis-Lieb solution of the Luttinger model [1, 2]. More recently, we found a new proof, based on the Ward identities obtained by a chiral local gauge transformation, applied to the Tomonaga model with infrared cutoff [3, 4]. This is an old approach in the physical literature, but its implementation in an RG scheme is not trivial at all, because the ultraviolet and infrared cutoffs destroy local gauge invariance and produce not negligible correction terms with respect to the formal Ward identities.

The solution of the problem is in the use of a new set of identities, called "Correction Identities", relating the corrections to the Schwinger functions and showing the phenomenon of *chiral anomaly*. By combining Ward and Correction identities with a Dyson equation, the vanishing of the Beta function follows, so that the infrared cutoff can be removed.

As a byproduct, even the ultraviolet cutoff can be removed, after a suitable ultraviolet renormalization, so that a Euclidean Quantum Field Theory corresponding to the Thirring model at imaginary time is constructed, for any value of the mass [5].

2 The Tomonaga Model with Infrared Cutoff

The model is not Hamiltonian and can be defined in terms of Grassmannian variables. It describes a system of two kinds of fermions with linear dispersion relation interacting with a local potential. Let $\mathcal{D}$ be the set of *space-time momenta* $\mathbf{k} = (k, k_0)$, with $k = \frac{2\pi}{L}(n + \frac{1}{2})$ and $k_0 = \frac{2\pi}{\beta}(n_0 + \frac{1}{2})$. With each $\mathbf{k} \in \mathcal{D}$ we associate four Grassmannian variables $\widehat{\psi}^{\sigma}_{\mathbf{k},\omega}$, $\sigma, \omega \in \{+, -\}$. The free model is described by the measure

$$P(d\psi) = \frac{\mathcal{D}\psi}{\mathcal{N}} \exp\left\{ -\frac{Z_0}{L\beta} \sum_{\substack{\omega=\pm 1 \\ \mathbf{k}\in\mathcal{D}}} C_{h,0}(\mathbf{k})(-ik_0 + \omega k)\widehat{\psi}^{+}_{\mathbf{k},\omega}\widehat{\psi}^{-}_{\mathbf{k},\omega} \right\} \tag{1}$$

where $\mathcal{N}$ is a normalization constant, $\mathcal{D}\psi$ is the *Lebesgue Grassmannian measure*, Z_0 is a fixed constant, that we shall put equal to 1, and $[C_{h,0}(\mathbf{k})]^{-1}$ is a smooth function, which has support in the interval $\{\gamma^{h-1} \le |\mathbf{k}| \le \gamma\}$, $\gamma > 1$, and is equal to 1 in the interval $\{\gamma^h \le |\mathbf{k}| \le 1\}$. The measure (1) is a *Gaussian Grassmannian measure* with propagator

$$\widehat{g}_{\omega}(\mathbf{k}) = \frac{1}{L\beta} \sum_{\mathbf{k}} \frac{[C_{h,0}(\mathbf{k})]^{-1}}{(-ik_0 + \omega k)}. \tag{2}$$

The correlation functions of density and field operators for the Tomonaga model with infrared cutoff can be obtained by the generating functional

$$\mathcal{W}(\phi, J) = \log \int P(d\psi) e^{-V(\psi)+\sum_\omega \int d\mathbf{x}\left[J_{\mathbf{x},\omega} Z_0^{(2)} \psi^+_{\mathbf{x},\omega}\psi^-_{\mathbf{x},\omega}+\phi^+_{\mathbf{x},\omega}\psi^-_{\mathbf{x},\omega}+\psi^+_{\mathbf{x},\omega}\phi^-_{\mathbf{x},\omega}\right]} \quad (3)$$

where

$$V(\psi) = \lambda (Z_0)^2 \int d\mathbf{x} \psi^+_{\mathbf{x},+}\psi^-_{\mathbf{x},+}\psi^+_{\mathbf{x},-}\psi^-_{\mathbf{x},-}, \quad Z_0^{(2)} = Z_0 = 1. \quad (4)$$

The correlation functions will be graphically represented as in the examples of Fig. 1. They are of course well defined, if γ^h is large enough; we want to discuss how to control the limit $h \to -\infty$.

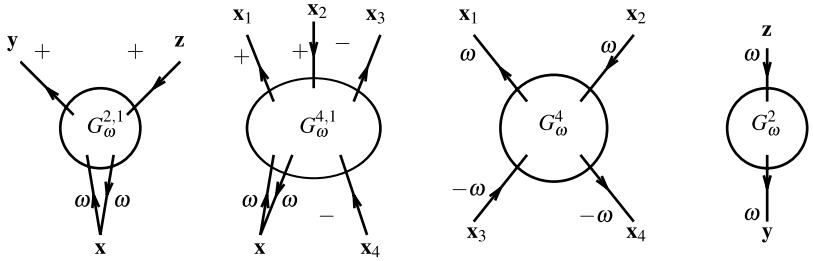

Fig. 1 Graphical representation of a few correlation functions

3 The RG Analysis

We shall perform a multi-scale analysis of the functional (3), by using the identity

$$[C_{h,0}(\mathbf{k})]^{-1} = \sum_{j=h}^{0} f_j(\mathbf{k}) \quad (5)$$

where the $f_j(\mathbf{k})$ are smooth functions defined so that

$$\text{supp}\, f_j(\mathbf{k}) = \{\gamma^{j-1} \le |\mathbf{k}| \le \gamma^{j+1}\}, \quad h \le j \le 0. \quad (6)$$

The decomposition (5) implies the following decomposition of the covariance (2) in *single scale covariances*:

$$\widehat{g}_\omega(\mathbf{k}) = \sum_{j=h}^{0} \widehat{g}^{(j)}_\omega(\mathbf{k}), \qquad \widehat{g}^{(j)}_\omega(\mathbf{k}) = \frac{1}{L\beta} \sum_{\mathbf{k}} \frac{f_j(\mathbf{k})}{(-ik_0 + \omega k)} \quad (7)$$

as well as a corresponding factorization of the measure (1) as the product of the Gaussian Grassmannian measures with propagators $\widehat{g}^{(j)}_\omega(\mathbf{k})$. Hence, we can perform iteratively the integration over the different scales, starting from $j = 0$. Moreover, after any integration step, we absorb in the remaining part of the free measure the terms linear in the momentum, so that at step j we get an expression of the type, see [4] for details:

$$e^{\mathcal{W}(\phi,J)} = e^{-L\beta E_j} \int P_{Z^{(h)}_j, C_{h,j}}(d\psi) e^{-V^{(j)}(\psi)+\mathcal{B}^{(j)}(\psi,\phi,J)} \tag{8}$$

where $P_{Z^{(h)}_j, C_{h,j}}$ has roughly the same form as (1), with the *field renormalization constant* $Z^{(h)}_j$ in place of Z_0, and the cutoff function

$$[C_{h,j}(\mathbf{k})]^{-1} = \sum_{i=h}^{j} f_j(\mathbf{k}) \tag{9}$$

in place of $[C_{h,0}(\mathbf{k})]^{-1}$; moreover,

$$V^{(j)}(\psi) = \lambda^{(h)}_j (Z^{(h)}_j)^2 \int d\mathbf{x}\, \psi^+_{\mathbf{x},+}\psi^-_{\mathbf{x},+}\psi^+_{\mathbf{x},-}\psi^-_{\mathbf{x},-} + \cdots \tag{10}$$

$$\mathcal{B}^{(j)}(\psi,\phi,J) = J_{\mathbf{x},\omega} Z^{(2,h)}_j \psi^+_{\mathbf{x},\omega}\psi^-_{\mathbf{x},\omega} + \phi^+_{\mathbf{x},\omega}\psi^-_{\mathbf{x},\omega} + \psi^+_{\mathbf{x},\omega}\phi^-_{\mathbf{x},\omega} + \cdots \tag{11}$$

where $\cdots$ denotes the remainder, made of irrelevant terms, $\lambda^{(h)}_j$ is the *running coupling* and $Z^{(2,h)}_j$ is the *density renormalization constant*.

Let us put $Z^{(1,h)}_j = Z^{(h)}_j$; it is easy to see, by using the definitions and the support properties of the single scale propagators, that, if $h' < h$,

$$\lambda^{(h')}_j = \lambda^{(h)}_j, \qquad Z^{(i,h')}_j = Z^{(i,h)}_j, \quad j = 0, \dots, h+1 \tag{12}$$

Moreover, one can show that, if we put $\varepsilon_h = \max_{0\le j\le h} |\lambda^{(h)}_j|$,

$$\lambda^{(h')}_h = \lambda^{(h)}_h + O(\varepsilon^2_h), \qquad Z^{(i,h')}_h / Z^{(i,h)}_h = 1 + O(\varepsilon^2_h). \tag{13}$$

Finally, if ε_h stays small for $h \to -\infty$, one can remove the infrared cutoff and show that [4]

$$\lambda_j \equiv \lambda^{(-\infty)}_j \xrightarrow[j\to-\infty]{} \lambda_{-\infty}(\lambda) \tag{14}$$

$$\frac{Z^{(i)}_{j-1}}{Z^{(i)}_j} \equiv \frac{Z^{(i,-\infty)}_{j-1}}{Z^{(i,-\infty)}_j} \longrightarrow j \to -\infty \eta_i(\lambda_{-\infty}) \tag{15}$$

$\lambda_{-\infty}(\lambda)$ and $\eta_i(\lambda_{-\infty})$ being analytic functions. Moreover $\lambda_{-\infty}(\lambda)$ is odd in λ and $\eta_i(\lambda_{-\infty})$ is even in $\lambda_{-\infty}$.

4 The Dyson Equation

To prove (14) is not an easy task, since the interaction is marginal, from the RG point of view, and indeed the bounds following from the RG analysis show a divergence linear in h. In order to clarify the origin of this apparent divergence and explain how to use Ward identities to solve the problem, it is convenient to consider the following Dyson equation:

$$-\widehat{G}^4_+(\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4)=\lambda\widehat{g}_-(\mathbf{k}_4)\Big[\widehat{G}^2_-(\mathbf{k}_3)\widehat{G}^{2,1}_+(\mathbf{k}_1-\mathbf{k}_2,\mathbf{k}_1,\mathbf{k}_2) + \frac{1}{L\beta}\sum_{\mathbf{p}} G^{4,1}_+(\mathbf{p};\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4-\mathbf{p})\Big] \tag{16}$$

whose graphical representation is given in Fig. 2.

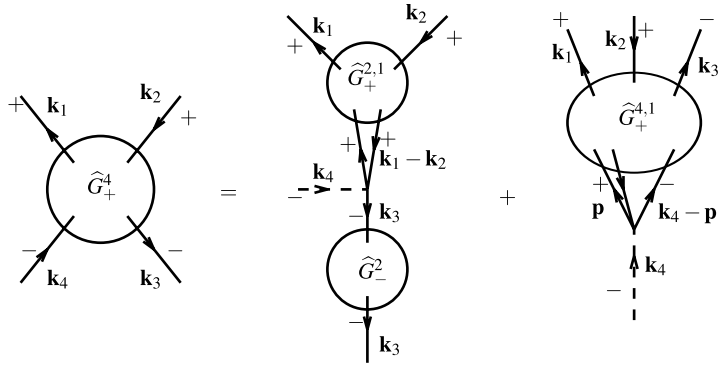

Fig. 2 Graphical representation of the Dyson equation (16)

The RG analysis allows us to get rigorously *dimensional bounds* on the correlation functions. In particular, if we fix the external momenta in the Dyson equation so that

$$\mathbf{k}_1=\mathbf{k}_4=-\mathbf{k}_2=-\mathbf{k}_3=\bar{\mathbf{k}},\quad |\bar{\mathbf{k}}|=\gamma^h \tag{17}$$

and ε_h is small enough, we get [3]

$$\widehat{G}^2_\omega(\bar{\mathbf{k}})=\frac{1}{Z^{(1,h)}_h D_\omega(\bar{\mathbf{k}})}[1+O(\varepsilon^2_h)],\quad D_\omega(\mathbf{k})=-ik_0+\omega k \tag{18}$$

$$\widehat{G}^{2,1}_\omega(2\bar{\mathbf{k}},\bar{\mathbf{k}},-\bar{\mathbf{k}})=-\frac{Z^{(2,h)}_h}{(Z^{(1,h)}_h)^2 D_\omega(\bar{\mathbf{k}})^2}[1+O(\varepsilon^2_h)] \tag{19}$$

$$\widehat{G}^4_+(\bar{\mathbf{k}},-\bar{\mathbf{k}},-\bar{\mathbf{k}},\bar{\mathbf{k}})=\frac{1}{(Z^{(1,h)}_h)^2|\bar{\mathbf{k}}|^4}[-\lambda^{(h)}_h+O(\varepsilon^2_h)]. \tag{20}$$

Then the l.h.s. of the Dyson equation is equal to

$$\frac{1}{(Z_h^{(1,h)})^2|\bar{\mathbf{k}}|^4}[\lambda_h^{(h)} + O(\varepsilon_h^2)] \tag{21}$$

while the first term in the r.h.s. is equal to

$$\frac{Z_h^{(2,h)}}{(Z_h^{(1,h)})^3|\bar{\mathbf{k}}|^4}\lambda[1 + O(\varepsilon_h^2)]. \tag{22}$$

As we shall explain below, by using the local gauge invariance of the interaction it is possible to show that

$$\frac{Z_h^{(2,h)}}{Z_h^{(1,h)}} = 1 + O(\varepsilon_h). \tag{23}$$

Were we able to bound the second term in the r.h.s. as

$$C\frac{\varepsilon_h^2}{(Z_h^{(1,h)})^2|\bar{\mathbf{k}}|^4} \tag{24}$$

then, by a simple iterative argument, we could prove that, if λ is small enough,

$$|\lambda_j^{(h)}| \le 2|\lambda|, \quad \forall h \text{ and } j \ge h \tag{25}$$

implying that the Tomonaga model is well defined.

However, the RG analysis only allows us to bound such term as

$$C\frac{\varepsilon_h}{(Z_h^{(1,h)})^2|\bar{\mathbf{k}}|^4}[\gamma^{C\varepsilon_h|h|} - 1] \tag{26}$$

which is of course not sufficient.

The natural guess is that the origin of the problem is in the fact that one is not taking into account some crucial cancellations related with the gauge invariance. Hence, inspired by the analysis in the physical literature [7], we rewrite $\widehat{G}_\omega^{4,1}$ in terms of $\widehat{G}_+^4$ by suitable *Ward identities*, that is the identities obtained by applying the *chiral gauge transformation*

$$\psi_{\mathbf{x},+}^{\pm} \to e^{\pm i\alpha_{\mathbf{x}}}\psi_{\mathbf{x},+}^{\pm}, \quad \psi_{\mathbf{x},-}^{\pm} \to \psi_{\mathbf{x},-}^{\pm} \tag{27}$$

in the generating functional.

As we shall discuss, this is not enough, because the corrections to the formal WI related with the cutoffs satisfy bounds of the same type of the previous one. The problem is finally solved by using other identities, which we call *correction identities*.

5 The First Ward Identity

By doing in (3) the chiral gauge transformation (27), one obtains [3] the Ward identity, see Fig. 3,

$$D_+(\mathbf{p})G_+^{2,1}(\mathbf{p},\mathbf{k},\mathbf{q}) = G_+^2(\mathbf{q}) - G_+^2(\mathbf{k}) + \Delta_+^{2,1}(\mathbf{p},\mathbf{k},\mathbf{q}). \tag{28}$$

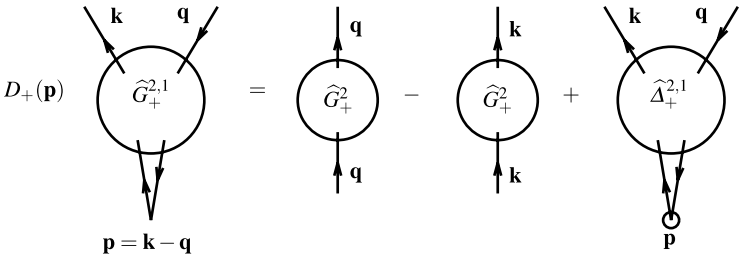

Fig. 3 Graphical representation of the Ward identity (28); the small circle in $\widehat{\Delta}_+^{2,1}$ represents the function C_+ of (30)

We used the definitions

$$\Delta_+^{2,1}(\mathbf{p},\mathbf{k},\mathbf{q}) = \frac{1}{\beta L}\sum_{\mathbf{k}} C_+(\mathbf{k},\mathbf{k}-\mathbf{p})\langle \widehat{\psi}^+_{\mathbf{k},+}\widehat{\psi}^-_{\mathbf{k}-\mathbf{p},+}; \widehat{\psi}^-_{\mathbf{k},+}\widehat{\psi}^+_{\mathbf{q},+}\rangle^T \tag{29}$$

and

$$C_\omega(\mathbf{k}^+,\mathbf{k}^-) = [C_{h,0}(\mathbf{k}^-)-1]D_\omega(\mathbf{k}^-) - [C_{h,0}(\mathbf{k}^+)-1]D_\omega(\mathbf{k}^+). \tag{30}$$

At graph level, the Ward identities follow from the trivial identity

$$\frac{1}{D_\omega(\mathbf{k})} - \frac{1}{D_\omega(\mathbf{k}+\mathbf{p})} = \frac{D_\omega(\mathbf{p})}{D_\omega(\mathbf{k})D_\omega(\mathbf{k}+\mathbf{p})}. \tag{31}$$

One could guess that the correction term $\Delta_+^{2,1}$ is negligible. However, this is not true, but we have the first correction identity where ν_+, ν_- are $O(\lambda)$ and weakly dependent on h. Moreover, the term $H_+^{2,1}$ is indeed negligible, in the sense that, if we can make the limit $h \to -\infty$, its contribution goes to 0 as the external momenta go to 0 (of course staying much larger than γ^h).

If we insert the correction identity in the WI, we get

$$\begin{aligned}(1-\nu_+)D_+(\mathbf{p})\widehat{G}_+^{2,1}(\mathbf{p},\mathbf{k},\mathbf{q}) - \nu_- D_-(\mathbf{p})\widehat{G}_-^{2,1}(\mathbf{p},\mathbf{k},\mathbf{q})\\ = \widehat{G}_+^2(\mathbf{q}) - \widehat{G}_+^2(\mathbf{k}) + \widehat{H}_+^{2,1}(\mathbf{p},\mathbf{k},\mathbf{q}).\end{aligned} \tag{32}$$

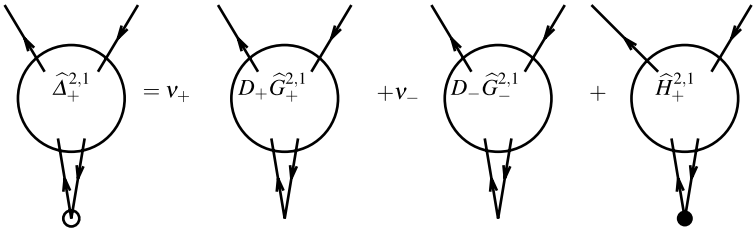

Fig. 4 The first Correction Identity; the filled point in the last term represents the function $C_+(\mathbf{k}, \mathbf{k}-\mathbf{p}) - \sum_\omega \nu_\omega D_\omega(\mathbf{p})$

The presence of $G^{2,1}_+$ in the correction identity is not a problem. In fact, this function satisfies another Ward identity and a corresponding correction identity, involving the same constants ν_+, ν_-, and we get

$$(1-\nu_+)D_-(\mathbf{p})\widehat{G}^{2,1}_-(\mathbf{p},\mathbf{k},\mathbf{q}) - \nu_- D_+(\mathbf{p})\widehat{G}^{2,1}_+(\mathbf{p},\mathbf{k},\mathbf{q}) = \widehat{H}^{2,1}_-(\mathbf{p},\mathbf{k},\mathbf{q}). \quad (33)$$

Hence, we can represent $\widehat{G}^{2,1}_+$ as a linear combination of propagators, as in the case of the formal WI, up to negligible terms.

The first WI can be used to prove that

$$\frac{Z^{(2)}_h}{Z^{(1)}_h} = 1 + O(\varepsilon_h). \quad (34)$$

In order to get this result, we put $\mathbf{k} = -\mathbf{q} = \bar{\mathbf{k}}$, with $|\bar{\mathbf{k}}| = \gamma^h$. For these values of the external momenta, $\widehat{H}^{2,1}_-(\mathbf{p},\mathbf{k},\mathbf{q})$ is not negligible, but one can show [3] that

$$\left|\frac{\widehat{\Delta}^{2,1}_+(2\bar{\mathbf{k}},\bar{\mathbf{k}},-\bar{\mathbf{k}})}{D_+(2\bar{\mathbf{k}})}\right| \le C\gamma^{-2h}\varepsilon_h \frac{Z^{(2)}_h}{(Z^{(1)}_h)^2}. \quad (35)$$

6 The Second Ward Identity

Another WI that plays an important role is that graphically represented in the following picture.

If one inserts this identity in the Dyson equation, the two terms containing the four point function give the right bound, but the correction term $\Delta^{4,1}_+/D_+(\mathbf{p})$ has the same bad bound as the original one, so making apparently useless the WI. However, there is again a correction identity, see Fig. 6, that allows us to solve this problem.

This identity involves also the correlation function $G^{4,1}_-$; hence, as before, in order to get a relation involving only $G^{4,1}_+$, G^4_+ and some *negligible* terms, one has to use also another WI and the corresponding correction identity.

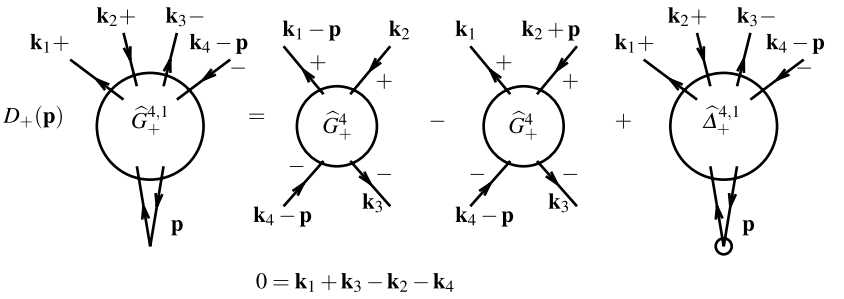

Fig. 5 The second Ward Identity; the small circle in the last term represents the function $C_+(\mathbf{k}, \mathbf{k}-\mathbf{p})$

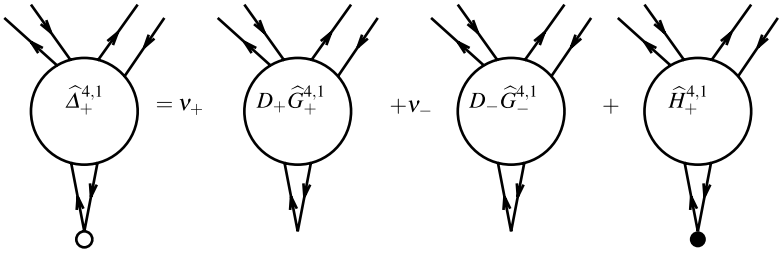

Fig. 6 The second Correction Identity; the filled point in the last term represents the function $C_+(\mathbf{k}, \mathbf{k}-\mathbf{p}) - \sum_\omega \nu_\omega D_\omega(\mathbf{p})$

However, to show that the contribution of $\widehat{H}^{4,1}_+$ has the right bound is not so simple, since we need to evaluate it for external momenta of order γ^h. It turns out that we have to evaluate a correlation very similar to the four point function with one of the external vertices substituted with a suitable "correction vertex", see [4] for the very technical details.

7 The Euclidean Thirring Model

It is a the Euclidean version of a relativistic two dimensional model, formally defined by the Grassmannian measure

$$d\bar{\psi}\, d\psi \exp\left\{-\int dx \left[-\bar{\psi}_x i\gamma^\mu \partial_\mu \psi_x + +\mu\bar{\psi}_x\psi_x + \lambda(\bar{\psi}_x\psi_x)^2\right]\right\} \tag{36}$$

$$\{\gamma^\mu, \gamma^\nu\} = -2\delta_{\mu,\nu}. \tag{37}$$

In order to give a meaning to the model, one has to introduce an u.v. and an i.r. cutoff, together with suitable field strength and interaction renormalization.

Let us consider the massless case, $\mu = 0$. By a suitable field transformation, one can show that the model can be written as the Tomonaga model with free measure

$$P(d\psi) = \frac{\mathcal{D}\psi}{\mathcal{N}} \exp\left\{ -\frac{Z_N^{(1)}}{L\beta} \sum_{\omega=\pm 1} \sum_{\mathbf{k}\in\mathcal{D}} C_{h,N}(\mathbf{k})(-ik_0 + \omega k)\widehat{\psi}_{\mathbf{k},\omega}\widehat{\psi}_{\mathbf{k},\omega} \right\}$$

and interaction

$$V(\psi) = \lambda_N \int d\mathbf{x}\ \psi^+_{\mathbf{x},+}\psi^-_{\mathbf{x},+}\psi^+_{\mathbf{x},-}\psi^-_{\mathbf{x},-}.$$

The Schwinger functions can be calculated by the generating functional

$$\mathcal{W}(\phi, J) = \log \int P(d\psi) e^{-V(\psi)+\sum_\omega \int d\mathbf{x}\left[J_{\mathbf{x},\omega} Z_N^{(2)} \psi^+_{\mathbf{x},\omega}\psi^-_{\mathbf{x},\omega} + \phi^+_{\mathbf{x},\omega}\psi^-_{\mathbf{x},\omega} + \psi^+_{\mathbf{x},\omega}\phi^-_{\mathbf{x},\omega}\right]}.$$

The analysis of the Tomonaga model implies that the cutoffs can be removed if

$$\lambda_N = \lambda\big(Z_N^{(1)}\big)^2$$
$$Z_N^{(1)} = c_1(\lambda)\gamma^{-N\eta(\lambda^*)}, \qquad Z_N^{(2)} = c_2(\lambda)\gamma^{-N\eta(\lambda^*)}, \quad \lambda^* = \lambda_{-\infty}(\lambda)$$

where $c_i(\lambda)$ are two arbitrary analytic functions such that $c_i(0)$ are strictly positive numbers. They have to be chosen by fixing the values of some correlations at finite values of their external momenta. Note that we have essentially already fixed the interaction strength at physical momentum scales of order one; it is given by λ^*.

In Ref. [5], which we refer to even for relevant references to the huge literature on the Thirring model, it is shown that all the field correlation functions are well defined, in the limit of removed cutoffs, and that they satisfy the Osterwalder–Schrader axioms. Hence, we are able to get results in agreement with known ones, obtained by different techniques. However, our approach can be extended, with a relatively minor effort, to the *massive* Thirring model ($\mu > 0$), which was up to now an open problem, at least from the point of view of Mathematical Physics.

In order to understand the type of results one can get, let us consider the two point function $S_\omega(\mathbf{k})$ in the massless case. Simple scaling arguments, based on the structure of its tree expansion after the cutoffs removal, imply that

$$S_\omega(\mathbf{k}) = \frac{|\mathbf{k}|^{\eta(\lambda^*)}}{D_\omega(\mathbf{k})} \frac{f(\lambda^*)}{c_1(\lambda)} \tag{38}$$

where $f(\lambda^*)$ is a suitable analytic function of λ^* (hence of λ), independent of $c_1(\lambda)$. If we put the renormalization condition

$$D_\omega(\mathbf{k})S_\omega(\mathbf{k}) = 1/m^\eta, \quad \text{if } |\mathbf{k}| = 1 \tag{39}$$

we get the well known formula

$$S_\omega(\mathbf{k}) = \frac{|\mathbf{k}/m|^{\eta(\lambda^*)}}{D_\omega(\mathbf{k})}. \tag{40}$$

Let us now consider the first WI for the Thirring model; we have

$$\frac{Z_N^{(1)}}{Z_N^{(2)}}\Big[(1-\nu_+)D_+(\mathbf{p})\widehat{G}_+^{2,1}(\mathbf{p},\mathbf{k},\mathbf{q}) - \nu_- D_-(\mathbf{p})\widehat{G}_-^{2,1}(\mathbf{p},\mathbf{k},\mathbf{q})\Big]$$
$$= \widehat{G}_+^2(\mathbf{q}) - \widehat{G}_+^2(\mathbf{k}) + \frac{Z_N^{(1)}}{Z_N^{(2)}}\widehat{H}_+^{2,1}(\mathbf{p},\mathbf{k},\mathbf{q}). \tag{41}$$

If we put $c_2(\lambda) = c_1(\lambda)$ and we remove the cutoffs, we get, for any non zero values of the external momenta

$$(1-\nu_+)D_+(\mathbf{p})\widehat{G}_+^{2,1}(\mathbf{p},\mathbf{k},\mathbf{q}) - \nu_- D_-(\mathbf{p})\widehat{G}_-^{2,1}(\mathbf{p},\mathbf{k},\mathbf{q}) = \widehat{G}_+^2(\mathbf{q}) - \widehat{G}_+^2(\mathbf{k}) \tag{42}$$

which shows the well known fact that the formal Ward identity is not satisfied, but *anomalous* terms are present, related to the non zero constants ν_+ and ν_-.

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New Algebraic Aspects of Perturbative and Non-perturbative Quantum Field Theory

Christoph Bergbauer and Dirk Kreimer

Abstract In this expository article we review recent advances in our understanding of the combinatorial and algebraic structure of perturbation theory in terms of Feynman graphs, and Dyson-Schwinger equations. Starting from Lie and Hopf algebras of Feynman graphs, perturbative renormalization is rephrased algebraically. The Hochschild cohomology of these Hopf algebras leads the way to Slavnov-Taylor identities and Dyson-Schwinger equations. We discuss recent progress in solving simple Dyson-Schwinger equations in the high energy sector using the algebraic machinery. Finally there is a short account on a relation to algebraic geometry and number theory: understanding Feynman integrals as periods of mixed (Tate) motives.

1 Introduction

As elements of perturbative expansions of Quantum field theories, Feynman graphs have been playing and still play a key role both for our conceptual understanding and for state-of-the-art computations in particle physics. This article is concerned with several aspects of Feynman graphs: First, the combinatorics of perturbative renormalization give rise to Hopf algebras of rooted trees and Feynman graphs. These Hopf algebras come with a cohomology theory and structure maps that help understand important physical notions, such as locality of counterterms, the beta function,

Christoph Bergbauer
Institut für Mathematik II, Freie Universität Berlin, Arnimallee 3, 14195 Berlin, Germany and Erwin-Schrödinger-Institut, Boltzmanngasse 9, 1090 Vienna, Austria, e-mail: bergbau@math.fu-berlin.de

Dirk Kreimer
CNRS at Institut des Hautes Etudes Scientifiques, 35 route de Chartres, 91440 Bures-sur-Yvette, France and Center for Mathematical Physics, Boston University, 111 Cummington Street, Boston, MA 02215, USA, e-mail: kreimer@ihes.fr

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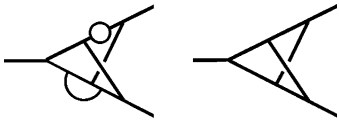
certain symmetries, or Dyson-Schwinger equations from a unified mathematical point of view. This point of view is about self-similarity and recursion. The atomic (primitive) elements in this combinatorial approach are divergent graphs without subdivergences. They must be studied by additional means, be it analytic methods or algebraic geometry and number theory, and this is a significantly more difficult task. However, the Hopf algebra structure of graphs for renormalization is in this sense a substructure of the Hopf algebra structure underlying the relative cohomology of graph hypersurfaces needed to understand the number-theoretic properties of field theory amplitudes [6, 5].

2 Lie and Hopf Algebras of Feynman Graphs

Given a Feynman graph Γ with several divergent subgraphs, the Bogoliubov recursion and Zimmermann's forest formula tell how Γ must be renormalized in order to obtain a finite conceptual result, using only local counterterms. This has an analytic (regularization/extension of distributions) and a combinatorial aspect. The basic *combinatorial* question of perturbative renormalization is to find a good model which describes disentanglement of graphs into subdivergent pieces, or dually insertion of divergent pieces one into each other, from the point of view of renormalized Feynman rules. It has been known now for several years that commutative Hopf algebras and (dual) Lie algebras provide such a framework [26, 14, 15] with many ramifications in pure mathematics. From the physical side, it is important to know that, for example, recovering aspects of gauge/BRST symmetry [40, 38, 31, 39] and the transition to nonperturbative equations of motion [11, 28, 29, 37, 3, 35, 32, 36, 4] are conveniently possible in this framework, as will be discussed in subsequent sections.

In order to introduce these Lie and Hopf algebras, let us now fix a renormalizable quantum field theory (in the sense of perturbation theory), given by a local Lagrangian. A convenient first example is massless ϕ^3 theory in 6 dimensions. We look at its perturbative expansion in terms of 1PI Feynman graphs. Each 1PI graph Γ comes with two integers, $|\Gamma| = |H_1(\Gamma)|$, its number of loops, and $\mathrm{sdd}(\Gamma)$, its superficial degree of divergence. As usual, vacuum and tadpole graphs need not be considered, and the only remaining superficial divergent graphs have exactly two or three external edges, a feature of renormalizability. Graphs without subdivergences are called *primitive*. Here are two examples.



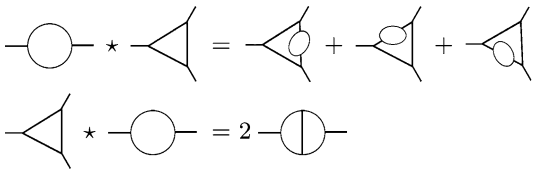
Both are superficially divergent as they have three external edges. The first one has two subdivergences, the second one is primitive. Note that there are infinitely many

primitive graphs with three external edges. In particular, for every $n \in \mathbb{N}$ one finds a primitive Γ such that $|\Gamma| = n$.

Let now L be the $\mathbb{Q}$-vector space generated by all the superficially divergent (sdd ≥ 0) 1PI graphs of our theory, graded by the number of loops $|\cdot|$. There is an operation on L given by insertion of graphs into each other: Let γ_1, γ_2 be two generators of L. Then

$$\gamma_1 \star \gamma_2 := \sum_{\Gamma} n(\gamma_1, \gamma_2, \Gamma)$$

where $n(\gamma_1, \gamma_2, \Gamma)$ is the number of times that γ_1 shows up as a subgraph of Γ and $\Gamma/\gamma_1 \cong \gamma_2$. Here are two examples:



This definition is extended bilinearly onto all of L. Note that $\star$ respects the grading as $|\gamma_1 \star \gamma_2| = |\gamma_1| + |\gamma_2|$. The operation $\star$ is not in general associative. Indeed, it is pre-Lie [14, 17]:

$$(\gamma_1 \star \gamma_2) \star \gamma_3 - \gamma_1 \star (\gamma_2 \star \gamma_3) = (\gamma_1 \star \gamma_3) \star \gamma_2 - \gamma_1 \star (\gamma_3 \star \gamma_3). \tag{1}$$

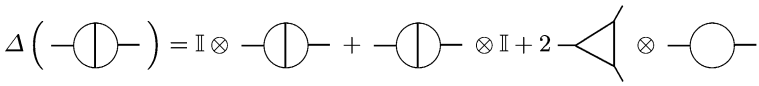
To see that (1) holds observe that on both sides nested insertions cancel. What remains are disjoint insertions of γ_2 and γ_3 into γ_1 which do obviously not depend on the order of γ_2 and γ_3. One defines a Lie bracket on L:

$$[\gamma_1, \gamma_2] := \gamma_1 \star \gamma_2 - \gamma_2 \star \gamma_1.$$

The Jacobi identity for $[\cdot, \cdot]$ is satisfied as a consequence of the pre-Lie property (1) of $\star$. This makes L a graded Lie algebra. The bracket is defined by mutual insertions of graphs. As usual, $\mathcal{U}(L)$, the universal enveloping algebra of L is a cocommutative Hopf algebra. Its graded dual, in the sense of Milnor-Moore, is therefore a commutative Hopf algebra $\mathcal{H}$. As an algebra, $\mathcal{H}$ is free commutative, generated by the vector space L and an adjoined unit $\mathbb{I}$. By duality, one expects the coproduct of $\mathcal{H}$ to disentangle its argument into subdivergent pieces. Indeed, one finds

$$\Delta(\Gamma) = \mathbb{I} \otimes \Gamma + \Gamma \otimes \mathbb{I} + \sum_{\gamma \subsetneq \Gamma} \gamma \otimes \Gamma/\gamma. \tag{2}$$

The relation $\gamma \subsetneq \Gamma$ refers to disjoint unions γ of 1PI superficially divergent subgraphs of Γ. Disjoint unions of graphs are in turn identified with their product in $\mathcal{H}$. For example,



The coproduct respects the grading by the loop number, as does the product (by definition). Therefore $\mathcal{H} = \bigoplus_{n=0}^{\infty} \mathcal{H}_n$ is a graded Hopf algebra. Since $\mathcal{H}_0 \cong \mathbb{Q}$ it is connected. The count ϵ vanishes on the subspace $\bigoplus_{n=1}^{\infty} \mathcal{H}_n$, called augmentation ideal, and $\epsilon(\mathbb{I}) = 1$. As usual, if $\Delta(x) = \mathbb{I} \otimes x + x \otimes \mathbb{I}$, the element x is called *primitive*. The linear subspace of primitive elements is denoted $\mathrm{Prim}\,\mathcal{H}$.

The interest in $\mathcal{H}$ and L arises from the fact that the Bogoliubov recursion is essentially solved by the antipode of $\mathcal{H}$. In any connected graded bialgebra, the antipode S is given by

$$S(x) = -x - \sum S(x')x'', \quad x \notin \mathcal{H}_0 \tag{3}$$

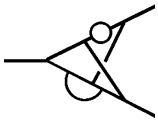
in Sweedler's notation. Let now V be a $\mathbb{C}$-algebra. The space of linear maps $\mathcal{L}_{\mathbb{Q}}(\mathcal{H}, V)$ is equipped with a convolution product $(f, g) \mapsto f * g = m_V(f \otimes g)\Delta$ where m_V is the product in V. Relevant examples for V are suggested by regularization schemes such as the algebra $V = \mathbb{C}[[\epsilon, \epsilon^{-1}]$ of Laurent series with finite pole part for dimensional regularization (space-time dimension $D = 6 + 2\epsilon$.) The (unrenormalized) Feynman rules provide then an algebra homomorphism $\phi : \mathcal{H} \to V$ mapping Feynman graphs to Feynman integrals in $6 + 2\epsilon$ dimensions. On V there is a linear endomorphism R (renormalization scheme) defined, for example minimal subtraction $R(\epsilon^n) = 0$ if $n \geq 0$, $R(\epsilon^n) = \epsilon^n$ if $n < 0$. If Γ is primitive, as defined above, then $\phi(\Gamma)$ has only a simple pole in ϵ, hence $(1 - R)\phi(\Gamma)$ is a good renormalized value for Γ. If Γ does have subdivergences, the situation is more complicated. However, the map $S_R^{\phi} : \mathcal{H} \to V$

$$S_R^{\phi}(\Gamma) = -R\left(\phi(\Gamma) - \sum S_R^{\phi}(\Gamma')\phi(\Gamma'')\right)$$

provides the counterterm prescribed by the Bogoliubov recursion, and $(S_R^{\phi} * \phi)(\Gamma)$ yields the renormalized value of Γ. The map S_R^{ϕ} is a recursive deformation of $\phi \circ S$ by R, compare its definition with (3). These are results obtained by one of the authors in collaboration with Connes [26, 14, 15].

For S_R^{ϕ} to be an algebra homomorphism again, one requires R to be a Rota-Baxter operator, studied in a more general setting by Ebrahimi-Fard, Guo and one of the authors in [20, 22, 21]. The Rota-Baxter property is at the algebraic origin of the Birkhoff decomposition introduced in [15, 16]. In the presence of mass terms, or gauge symmetries etc. in the Lagrangian, ϕ, S_R^{ϕ} and $S_R^{\phi} \star \phi$ may contribute to several form factors in the usual way. This can be resolved by considering a slight extension of the Hopf algebra containing projections onto single structure functions, as discussed for example in [15, 32]. For the case of gauge theories, a precise definition of the coefficients $n(\gamma_1, \gamma_2, \Gamma)$ is given in [31].

The Hopf algebra $\mathcal{H}$ arises from the simple insertion of graphs into each other in a completely canonical way. Indeed, the pre-Lie product determines the coproduct, and the coproduct determines the antipode. Like this, each quantum field theory gives rise to such a Hopf algebra $\mathcal{H}$ based on its 1PI graphs. It is no surprise then that there is an even more universal Hopf algebra behind all of them: The Hopf algebra $\mathcal{H}_{rt}$ of rooted trees [26, 14]. In order to see this, imagine a purely nested situation of subdivergences like

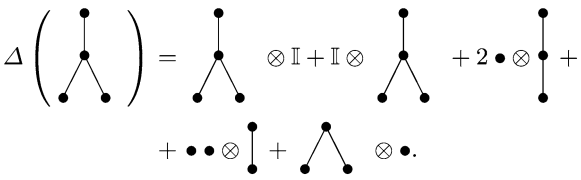


which can be represented by the rooted tree

To account for each single graph of this kind, the tree's vertices should actually be labeled according to which primitive graph they correspond to (plus some gluing data) which we will suppress for the sake of simplicity. The coproduct on $\mathcal{H}_{rt}$—corresponding to the one (2) of $\mathcal{H}$—is

$$\Delta(\tau) = \mathbb{I} \otimes \tau + \tau \otimes \mathbb{I} + \sum_{adm.c} P_c(\tau) \otimes R_c(\tau)$$

where the sum runs over all *admissible cuts* of the tree τ. A cut of τ is a nonempty subset of its edges which are to be removed. A cut $c(\tau)$ is defined to be admissible, if for each leaf l of τ at most one edge on the path from l to the root is cut. The product of subtrees which fall down when those edges are removed is denoted $P_c(\tau)$. The part which remains connected with the root is denoted $R_c(\tau)$. Here is an example:



Compared to $\mathcal{H}_{rt}$, the advantage of $\mathcal{H}$ is however that overlapping divergences are resolved automatically. To achieve this in $\mathcal{H}_{rt}$ requires some care [27].

3 From Hochschild Cohomology to Physics

There is a natural cohomology theory on $\mathcal{H}$ and $\mathcal{H}_{rt}$ whose non-exact 1-cocycles play an important "operadic" role in the sense that they drive the recursion that define the full 1PI Green's functions in terms of primitive graphs. In order to introduce this cohomology theory, let A be any bialgebra. We view A as a bicomodule over itself with right coaction $(id \otimes \epsilon)\Delta$. Then the Hochschild cohomology of A (with respect to the coalgebra part) is defined as follows [14]: Linear maps $L : A \to A^{\otimes n}$ are considered as n-cochains. The operator b, defined as

$$bL := (id \otimes L)\Delta + \sum_{i=1}^{n} (-1)^i \Delta_i L + (-1)^{n+1} L \otimes \mathbb{I} \tag{4}$$

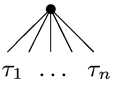
furnishes a codifferential: $b^2 = 0$. Here Δ denotes the coproduct of A and Δ_i the coproduct applied to the i-th factor in $A^{\otimes n}$. The map $L \otimes \mathbb{I}$ is given by $x \mapsto L(x) \otimes \mathbb{I}$. Clearly this codifferential encodes only information about the *coalgebra* (as opposed to the algebra) part of A. The resulting cohomology is denoted $\mathrm{HH}^\bullet_\epsilon(A)$. For $n = 1$, the cocycle condition $bL = 0$ is simply

$$\Delta L = (id \otimes L)\Delta + L \otimes \mathbb{I} \tag{5}$$

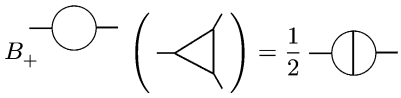
for L a linear endomorphism of A. In the Hopf algebra $\mathcal{H}_{rt}$ of rooted trees (where things are often simpler), a 1-cocycle is quickly found: the grafting operator B_+, defined by

$$B_+(\mathbb{I}) = \bullet$$

$$B_+(\tau_1 \dots \tau_n) = \quad \text{for trees } \tau_i$$



joining all the roots of its argument to a newly created root. Clearly, B_+ reminds of an operad multiplication. It is easily seen that B_+ is not exact and therefore a generator (among others) of $\mathrm{HH}^1_\epsilon(\mathcal{H}_{rt})$. Foissy [23, 24] showed that $L \mapsto L(\mathbb{I})$ is an onto map $\mathrm{HH}^1_\epsilon(\mathcal{H}_{rt}) \to \mathrm{Prim}\,\mathcal{H}_{rt}$. The higher Hochschild cohomology ($n \geq 2$) of $\mathcal{H}_{rt}$ is known to vanish [23, 24]. The pair $(\mathcal{H}_{rt}, B_+)$ is the universal model for all Hopf algebras of Feynman graphs and their 1-cocycles [14]. Let us now turn to those 1-cocycles of $\mathcal{H}$. Clearly, every primitive graph γ gives rise to a 1-cocycle B^γ_+ defined as the operator which inserts its argument, a product of graphs, into γ in all possible ways. Here is a simple example:



See [31] for the general definition involving some combinatorics of insertion places and symmetries.

It is an important consequence of the B_+^γ satisfying the cocycle condition (5) that

$$(S_R^\phi * \phi) B_+ = (1 - R)\tilde{B}_+(S_R^\phi * \phi) \tag{6}$$

where $\tilde{B}_+$ is the push-forward of B_+ along the Feynman rules ϕ. In other words, $\tilde{B}_+^\gamma$ is the integral operator corresponding to the skeleton graph γ. This is the combinatorial key to the proof of locality of counterterms and finiteness of renormalization [13, 28, 2, 3]. Indeed, (6) says that after treating all subdivergences, an overall subtraction $(1 - R)$ suffices. The only analytic ingredient is Weinberg's theorem applied to the primitive graphs. In [2] it is emphasized that $\mathcal{H}$ is actually generated (and determined) by the action of prescribed 1-cocycles and the multiplication. A version of (6) with decorated trees is available which describes renormalization in coordinate space [2].

The 1-cocycles B_+^γ give rise to a number of useful Hopf subalgebras of $\mathcal{H}$. Many of them are isomorphic. They are studied in [3] on the model of decorated rooted trees, and we will come back to them in the next section. In [31] one of the authors showed that in non-Abelian gauge theories, the existence of a certain Hopf subalgebra, generated by 1-cocycles, is closely related to the Slavnov-Taylor identities for the couplings to hold. In a similar spirit, van Suijlekom showed that, in QED, Ward-Takahashi identities, and in non-Abelian Yang-Mills theories, the Slavnov-Taylor identities for the couplings generate Hopf ideals $\mathcal{I}$ of $\mathcal{H}$ such that the quotients $\mathcal{H}/\mathcal{I}$ are defined and the Feynman rules factor through them [38, 39]. The Hopf algebra $\mathcal{H}$ for QED had been studied before in [10, 34, 40].

4 Dyson-Schwinger Equations

The ultimate application of the Hochschild 1-cocycles introduced in the previous section aims at non-perturbative results. Dyson-Schwinger equations, reorganized using the correspondence $\operatorname{Prim}\mathcal{H} \to \mathrm{HH}_\epsilon^1(\mathcal{H})$, become recursive equations in $\mathcal{H}[[\alpha]]$, α the coupling constant, with contributions from (degree 1) 1-cocycles. The Feynman rules connect them to the usual integral kernel representation. We remain in the massless ϕ^3 theory in 6 dimensions for the moment. Let $\Gamma^\perp$ be the *full* 1PI vertex function,

$$\Gamma = \mathbb{I} + \sum_{\operatorname{res}\Gamma = \perp} \alpha^{|\Gamma|} \frac{\Gamma}{\operatorname{Sym}\Gamma} \tag{7}$$

(normalized such that the tree level contribution equals 1). This is a formal power series in α with values in $\mathcal{H}$. Here $\operatorname{res}\Gamma$ is the result of collapsing all internal lines of Γ. The graph $\operatorname{res}\Gamma$ is called the residue of Γ. In a renormalizable theory, res can be seen as a map from the set of generators of $\mathcal{H}$ to the terms in the Lagrangian. For instance, in the ϕ^3 theory, vertex graphs have residue $\perp$, and self energy graphs have residue $-$. The number $\operatorname{Sym}\Gamma$ denotes the order of the group of automorphisms of Γ, defined in detail for example in [31, 39]. Similarly, the *full* inverse propagator

Γ^- is represented by

$$\Gamma^- = \mathbb{I} - \sum_{\text{res}\,\Gamma=-} \alpha^{|\Gamma|} \frac{\Gamma}{\text{Sym}\,\Gamma}. \tag{8}$$

These series can be reorganized by summing only over primitive graphs, with all possible insertions into these primitive graphs. In $\mathcal{H}$, the insertions are afforded by the corresponding Hochschild 1-cocycles. Indeed,

$$\begin{aligned} \Gamma^\perp &= \mathbb{I} + \sum_{\gamma\in\text{Prim}\,\mathcal{H},\text{res}\,\gamma=\perp} \frac{\alpha^{|\gamma|} B_+^\gamma(\Gamma^\perp Q^{|\gamma|})}{\text{Sym}\,\gamma} \\ \Gamma^- &= \mathbb{I} - \sum_{\gamma\in\text{Prim}\,\mathcal{H},\text{res}\,\gamma=-} \frac{\alpha^{|\gamma|} B_+^\gamma(\Gamma^- Q^{|\gamma|})}{\text{Sym}\,\gamma}. \end{aligned} \tag{9}$$

The universal invariant charge Q is a monomial in the Γ^r and their inverses, where r are residues (terms in the Lagrangian) provided by the theory. In ϕ^3 theory we have $Q = (\Gamma^\perp)^2(\Gamma^-)^{-3}$. In ϕ^3 theory, the universality of Q (i.e. the fact that the same Q is good for *all* Dyson-Schwinger equations of the theory) comes from a simple topological argument. In non-Abelian gauge theories however, the universality of Q takes care that the solution of the corresponding system of coupled Dyson-Schwinger equations gives rise to a Hopf subalgebra and therefore amounts to the Slavnov-Taylor identities for the couplings [31].

The system (9) of coupled Dyson-Schwinger equations has (7,8) as its solution. Note that in the first equation of (9) an *infinite* number of cocycles contributes as there are infinitely many primitive vertex graphs in ϕ_6^3 theory—the second equation has only finitely many contributions—here one. Before we describe how to actually attempt to solve equations of this kind analytically (application of the Feynman rules ϕ), we discuss the combinatorial ramifications of this construction in the Hopf algebra. It makes sense to call all (systems of) recursive equations of the form

$$\begin{aligned} X_1 &= \mathbb{I} \pm \sum_n \alpha^{k_n^1} B_+^{d_n^1}(M_n^1) \\ &\cdots \\ X_s &= \mathbb{I} \pm \sum_n \alpha^{k_n^s} B_+^{d_n^s}(M_n^s) \end{aligned}$$

combinatorial Dyson-Schwinger equations, and to study their combinatorics. Here, the $B_+^{d_n}$ are non-exact Hochschild 1-cocycles and the M_n are monomials in the $X_1 \dots X_s$. In [3] we studied a large class of single (uncoupled) combinatorial Dyson-Schwinger equations in a decorated version of $\mathcal{H}_{rt}$ as a model for vertex insertions:

$$X = \mathbb{I} + \sum_{n=1}^{\infty} \alpha^n w_n B_+^{d_n}(X^{n+1})$$

where the $w_n \in \mathbb{Q}$. For example, $X = \mathbb{I} + \alpha B_+(X^2) + \alpha^2 B_+(X^3)$ is in this class. It turns out [28, 3] that the coefficients c_n of X, defined by $X = \sum_{n=0}^{\infty} \alpha^n c_n$ generate a Hopf subalgebra themselves:

$$\Delta(c_n) = \sum_{k=0}^{n} P_k^n \otimes c_k.$$

The P_k^n are homogeneous polynomials of degree $n - k$ in the c_l, $l \leq n$. These polynomials have been worked out explicitly in [3]. One notices in particular that the P_k^n are independent of the w_n and $B_+^{d_n}$, and hence that under mild assumptions (on the algebraic independence of the c_n) the Hopf subalgebras generated this way are actually isomorphic. For example, $X = \mathbb{I} + \alpha B_+(X^2) + \alpha^2 B_+(X^3)$ and $X = \mathbb{I} + \alpha B_+(X^2)$ yield isomorphic Hopf subalgebras. This is an aspect of the fact that *truncation* of Dyson-Schwinger equations—considering only a finite instead of an infinite number of contributing cocycles—does make (at least combinatorial) sense. Indeed, the combinatorics remain invariant. Similar results hold for Dyson-Schwinger equations in the true Hopf algebra of graphs $\mathcal{H}$ where things are a bit more difficult though as the cocycles there involve some bookkeeping of insertion places.

The simplest nontrivial Dyson-Schwinger equation one can think of is the *linear* one:

$$X = \mathbb{I} + \alpha B_+(X).$$

Its solution is given by $X = \sum_{n=0}^{\infty} \alpha^n (B_+)^n(\mathbb{I})$. In this case X is grouplike and the corresponding Hopf subalgebra of c_ns is *cocommutative* [33]. A typical and important *non-linear* Dyson-Schwinger equation arises from propagator insertions:

$$X = \mathbb{I} - \alpha B_+(1/X),$$

for example the massless fermion propagator in Yukawa theory where only the fermion line obtains radiative corrections (other corrections are ignored). This problem has been studied and solved by Broadhurst and one of the authors in [11] and revisited recently by one of the authors and Yeats [35]. As we now turn to the analytic aspects of Dyson-Schwinger equations, we briefly sketch the general approach presented in [35] on how to successfully treat the nonlinearity of Dyson-Schwinger equations. Indeed, the *linear* Dyson-Schwinger equations can be solved by a simple scaling ansatz [33]. In any case, let γ be a primitive graph. The following works for amplitudes which depend on a single scale, so let us assume a massless situation with only one non-zero external momentum—how more than one external momentum (vertex insertions) are incorporated by enlarging the set of primitive elements is sketched in [32]. The grafting operator B_+^γ associated to γ translates to an integral operator under the (renormalized) Feynman rules

$$\phi_R(B_+^\gamma)(\mathbb{I})(p^2/\mu^2) = \int (I_\gamma(k, p) - I_\gamma(k, \mu))dk$$

where I_γ is the integral kernel corresponding to γ, the internal momenta are denoted by k, the external momentum by p, and μ is the fixed momentum at which we subtract: $R(x) = x|_{p^2=\mu^2}$.

In the following we stick to the special case discussed in [35] where only *one* internal edge is allowed to receive corrections. The integral kernel $\phi(B_+^\gamma)$ defines a Mellin transform

$$F(\rho) = \int I_\gamma(k,\mu)(k_i^2)^{-\rho} dk$$

where k_i is the momentum of the internal edge of γ at which insertions may take place (here the fermion line). If there are several insertion sites, obvious multiple Mellin transforms become necessary. The case of two (propagator) insertion places has been studied, at the same example, in [35].

The function $F(\rho)$ has a simple pole in ρ at 0. We write

$$F(\rho) = \frac{r}{\rho} + \sum_{n=0}^{\infty} f_n \rho^n.$$

We denote $L = \log p^2/\mu^2$. Clearly $\phi_R(X) = 1 + \sum_n \gamma_n L^n$. An important result of [35] is that, even in the difficult nonlinear situation, the anomalous dimension γ_1 is implicitly defined by the residue r and Taylor coefficients f_n of the Mellin transform F. On the other hand, all the γ_n for $n \geq 2$, are recursively defined in terms of the γ_i, $i < n$. This last statement amounts to a renormalization group argument that is afforded in the Hopf algebra by the scattering formula of [16]. Curiously, for this argument only a linearized part of the coproduct is needed. We refer to [35] for the actual algorithm. For a *linear* Dyson-Schwinger equation, the situation is considerably simpler as the $\gamma_n = 0$ for $n \geq 2$ since X is grouplike [33].

Let us restate the results for the high energy sector of non-linear Dyson-Schwinger equations [11, 35]: Primitive graphs γ define Mellin transforms via their integral kernels $\tilde{B}_+^\gamma$. The anomalous dimension γ_1 is *implicitly* determined order by order from the coefficients of those Mellin transforms. All non-leading log coefficients γ_n are recursively determined by γ_1, thanks to the renormalization group. This reduces, in principle, the problem to a study of all the primitive graphs and the intricacies of insertion places.

Finding useful representations of those Mellin transforms—even one-dimensional ones—of higher loop order skeleton graphs is difficult. However, the two-loop primitive vertex in massless Yukawa theory has been worked out by Bierenbaum, Weinzierl and one of the authors in [4], a result that can be applied to other theories as well. Combined with the algebraic treatment [11, 3, 35] sketched in the previous paragraphs and new geometric insight on primitive graphs (see Sect. 5), there is reasonable hope that actual solutions of Dyson-Schwinger equations will be more accessible in the future.

Using the Dyson-Schwinger analysis, one of the authors and Yeats [36] were able to deduce a bound for the convergence of superficially divergent amplitudes/structure functions from the (desirable) existence of a bound for the superficially convergent amplitudes.

5 Feynman Integrals and Periods of Mixed (Tate) Hodge Structures

A primitive graph $\Gamma \in \operatorname{Prim}\mathcal{H}$ defines a real number r_Γ, called the *residue* of Γ, which is independent of the renormalization scheme. In the case that Γ is massless and has one external momentum p, the residue r_Γ is the coefficient of $\log p^2/\mu^2$ in $\phi_R(\Gamma) = (1 - R)\phi(\Gamma)$. It coincides with the coefficient r of the Mellin transform introduced in the previous section. One may ask what kind of a number r is, for example if it is rational or algebraic. The origin of this question is that the irrational or transcendental numbers that show up for various Γ strongly suggest a motivic interpretation of the r_Γ. Indeed, explicit calculations [8, 9, 12] display patterns of Riemann zeta and multiple zeta values that are known to be periods of mixed Tate Hodge structures—here the periods are provided by the Feynman rules which produce $\Gamma \mapsto r_\Gamma$. By disproving a related conjecture of Kontsevich, Belkale and Brosnan [1] have shown that not all these Feynman motives must be mixed Tate, so one may expect a larger class of Feynman periods than multiple zeta values. Our detailed understanding of these phenomena is still far from complete, and only some very first steps have been made in the last few years. However, techniques developed in recent work by Bloch, Esnault and one of the authors [7] do permit reasonable insight for some special cases which we briefly sketch in the following.

Let Γ be a logarithmically divergent massless primitive graph with one external momentum p. It is convenient to work in the "Schwinger" parametric representation [25] obtained by the usual trick of replacing propagators

$$\frac{1}{k^2} = \int_0^\infty da e^{-ak^2},$$

and performing the loop integrations (Gaussian integrals) first which leaves us with a (divergent) integral over various Schwinger parameters a. It is a classical exercise [25, 7, 6] to show that in four dimensions, up to some powers of i and 2π,

$$\phi(\Gamma) = \int_0^\infty da_1 \cdots da_n \frac{e^{-Q_\Gamma(a,p^2)/\Psi_\Gamma(a)}}{\Psi_\Gamma^2(a)}$$

where n is the number of edges of Γ. Q_Γ and Ψ_Γ are graph polynomials of Γ, where Ψ_Γ, sometimes called *Symanzik* or *Kirchhoff polynomial*, is defined as follows: Let $T(\Gamma)$ be the set of spanning trees of Γ, i.e. the set of connected simply connected subgraphs which meet all vertices of Γ. We think of the edges e of Γ as being numbered from 1 to n. Then

$$\Psi_\Gamma = \sum_{t \in T(\Gamma)} \prod_{e \notin t} a_e.$$

This is a homogeneous polynomial in the a_i of degree $|H_1(\Gamma)|$. It is easily seen (scaling behaviour of Q_Γ and Ψ_Γ) that $r_\Gamma = \frac{\partial \phi_R(\Gamma)}{\partial \log p^2/\mu^2}$ is extracted from $\phi(\Gamma)$

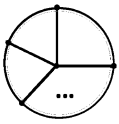
by considering the a_i as homogeneous coordinates of $\mathbb{P}^{n-1}(\mathbb{R})$ and evaluating at $p^2 = 0$:

$$r_\Gamma = \int_{\sigma \subset \mathbb{P}^{n-1}(\mathbb{R})} \frac{\Omega}{\Psi_\Gamma^2} \tag{10}$$

where $\sigma = \{[a_1, \ldots, a_n]$: all a_i can be chosen $\geq 0\}$ and Ω is a volume form on $\mathbb{P}^{n-1}$. Let $X_\Gamma := \{\Psi_\Gamma = 0\} \subset \mathbb{P}^{n-1}$. If $|H_1(\Gamma)| = 1$, the integrand in (10) has no poles. If $|H_1(\Gamma)| > 1$, poles will show up on the union $\Delta = \bigcup_{\gamma \subsetneq \Gamma, H_1(\gamma) \neq 0} L_\gamma$ of coordinate linear spaces $L_\gamma = \{a_e = 0$ for e edge of $\gamma\}$—these need to be separated from the chain of integration by blowing up. The blowups being understood, the Feynman motive is, by abuse of notation,

$$H^{n-1}(\mathbb{P}^{n-1} - X_\Gamma, \Delta - \Delta \cap X_\Gamma)$$

with Feynman period given by (10). See [7, 6] for details. Some particularly accessible examples are the *wheel with n spokes graphs*

$\Gamma_n :=$ 

studied extensively in [7]. The corresponding Feynman periods (10) yield rational multiples of zeta values [8]

$$r_{\Gamma_n} \in \zeta(2n-3)\mathbb{Q}.$$

Due to the simple topology of the Γ_n, the geometry of the pairs $(X_{\Gamma_n}, \Delta_{\Gamma_n})$ are well understood and the corresponding motives have been worked out explicitly [7]. The methods used are however nontrivial and not immediately applicable to more general situations.

When confronted with non-primitive graphs, i.e. graphs with subdivergences, there are more than one period to consider. In the Schwinger parameter picture, subdivergences arise when poles appear along exceptional divisors as pieces of Δ are blown up. This situation can be understood using limiting mixed Hodge structures [6], see also [30, 37] for a toy model approach to the combinatorics involved. In [6] it is also shown how the Hopf algebra $\mathcal{H}$ of graphs lifts to the category of motives. For the motivic role of solutions of Dyson-Schwinger equations we refer to work in progress. Finally we mention that there is related work by Connes and Marcolli [18, 19] who attack the problem via Riemann-Hilbert correspondences and motivic Galois theory.

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Exact Solution of the Six-Vertex Model with Domain Wall Boundary Conditions

Pavel M. Bleher*

Abstract The six-vertex model, or the square ice model, with domain wall boundary conditions (DWBC) has been introduced and solved for finite N by Korepin and Izergin. The solution is based on the Yang-Baxter equations and it represents the free energy in terms of an $N \times N$ Hankel determinant. Paul Zinn-Justin observed that the Izergin-Korepin formula can be re-expressed in terms of the partition function of a random matrix model with a nonpolynomial interaction. We use this observation to obtain the large N asymptotics of the six-vertex model with DWBC in the disordered phase and ferroelectric phases, and also on the critical line between these two phases. The solution is based on the Riemann-Hilbert approach.

1 Six-Vertex Model

The *six-vertex model*, or the model of *two-dimensional ice*, is stated on a square lattice with arrows on edges. The arrows obey the rule that at every vertex there are two arrows pointing in and two arrows pointing out. Such rule is sometimes called the ice-rule. There are only six possible configurations of arrows at each vertex, hence the name of the model, see Fig. 1.

We will consider the *domain wall boundary conditions* (DWBC), in which the arrows on the upper and lower boundaries point in the square, and the ones on the left and right boundaries point out. One possible configuration with DWBC on the 4×4 lattice is shown on Fig. 2.

The name of the *square ice* comes from the two-dimensional arrangement of water molecules, H_2O, with oxygen atoms at the vertices of the lattice and one

Pavel M. Bleher
Department of Mathematical Sciences, Indiana University-Purdue University Indianapolis, 402 N. Blackford St., Indianapolis, IN 46202, USA, e-mail: bleher@math.iupui.edu

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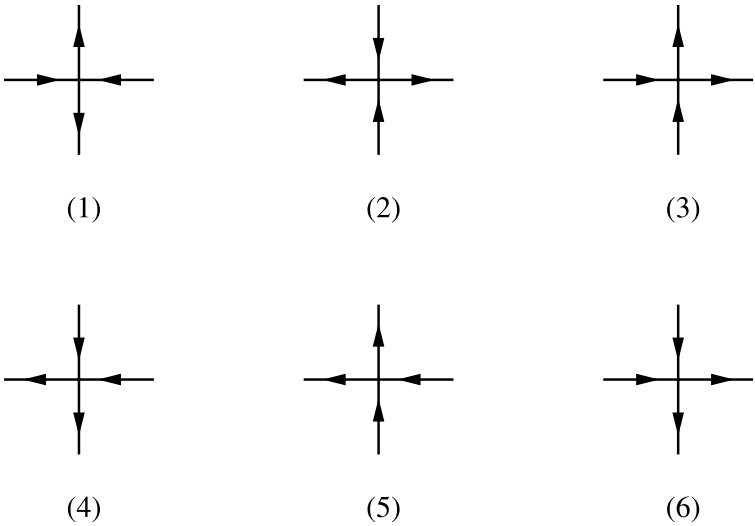

Fig. 1 The six arrow configurations allowed at a vertex

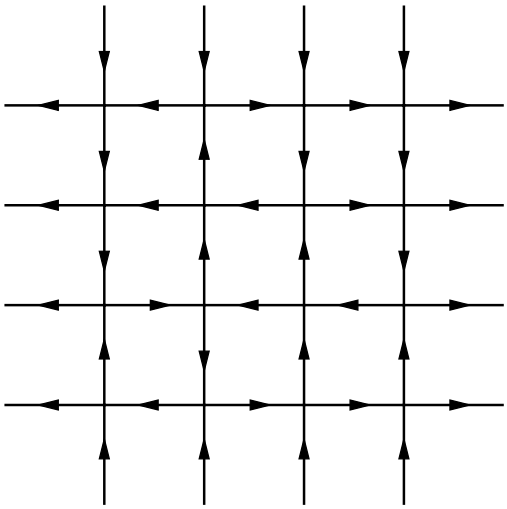

Fig. 2 An example of 4×4 configuration

hydrogen atom between each pair of adjacent oxygen atoms. We place an arrow in the direction from a hydrogen atom toward an oxygen atom if there is a bond between them. Thus, as we already noticed before, there are two in-bound and two out-bound arrows at each vertex.

For each possible vertex state we assign a *weight* w_i, $i = 1, \dots, 6$, and define, as usual, the *partition function*, as a sum over all possible arrow configurations of the product of the vertex weights,

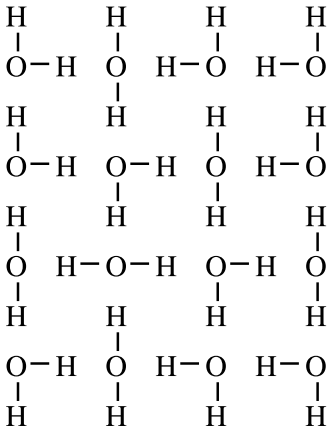

Fig. 3 The corresponding ice model

$$Z_N = \sum_{\text{arrow configurations } \sigma} w(\sigma), \qquad w(\sigma) = \prod_{x \in V_N} w_{\sigma(x)} = \prod_{i=1}^{6} w_i^{N_i(\sigma)}, \tag{1}$$

where V_N is the $N \times N$ set of vertices, $\sigma(x) \in \{1, \ldots, 6\}$ is the vertex configuration of σ at vertex x, according to Fig. 1, and $N_i(\sigma)$ is the number of vertices of type i in the configuration σ. The sum is taken over all possible configurations obeying the given boundary condition. The *Gibbs measure* is defined then as

$$\mu_N(\sigma) = \frac{w(\sigma)}{Z_N}. \tag{2}$$

Our main goal is to obtain the *large N asymptotics* of the partition function Z_N.

In general, the six-vertex model has *six parameters*: the weights w_i. However, by using some conservation laws we can reduce these to only *two parameters*. Namely, first we reduce to the case

$$w_1 = w_2 \equiv a, \qquad w_3 = w_4 \equiv b, \qquad w_5 = w_6 \equiv c, \tag{3}$$

and then, by using the identity,

$$Z_N(a, a, b, b, c, c) = c^{N^2} Z_N\left(\frac{a}{c}, \frac{a}{c}, \frac{b}{c}, \frac{b}{c}, 1, 1\right), \tag{4}$$

to the two parameters, $\frac{a}{c}$ and $\frac{b}{c}$. For details on how we make this reduction, see, e.g., the works [1] of Allison and Reshetikhin, [11] of Ferrari and Spohn, and [7] of Bleher and Liechty.

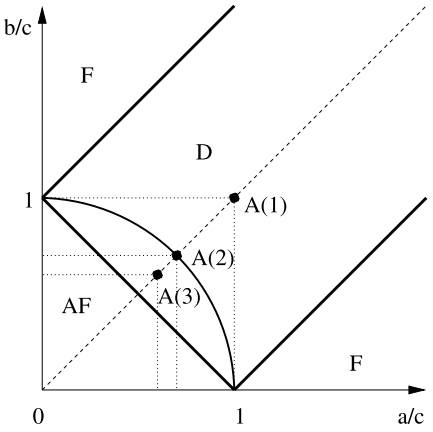

Fig. 4 The phase diagram of the model, where **F**, **AF** and **D** mark ferroelectric, antiferroelectric, and disordered phases, respectively. The circular arc corresponds to the so-called "free fermion" line, where $\Delta = 0$, and the three dots correspond to 1-, 2-, and 3-enumeration of alternating sign matrices

2 Phase Diagram of the Six-Vertex Model

Introduce the parameter

$$\Delta = \frac{a^2 + b^2 - c^2}{2ab}. \tag{5}$$

The *phase diagram* of the six-vertex model consists of the following three regions: the *ferroelectric phase region*, $\Delta > 1$; the *anti-ferroelectric phase region*, $\Delta < -1$; and, the *disordered phase region*, $-1 < \Delta < 1$, see, e.g., [21]. In these three regions we parameterize the weights in the standard way: in the ferroelectric phase region,

$$a = \sinh(t-\gamma), \qquad b = \sinh(t+\gamma), \qquad c = \sinh(2|\gamma|), \qquad 0 < |\gamma| < t, \tag{6}$$

in the anti-ferroelectric phase region,

$$a = \sinh(\gamma - t), \qquad b = \sinh(\gamma + t), \qquad c = \sinh(2\gamma), \qquad |t| < \gamma, \tag{7}$$

and in the disordered phase region,

$$a = \sin(\gamma - t), \qquad b = \sin(\gamma + t), \qquad c = \sin(2\gamma), \qquad |t| < \gamma. \tag{8}$$

The phase diagram of the model is shown on Fig. 4.

Here we will discuss the disordered and ferroelectric phase regions, and we will use parameterizations (8) and (6).

The phase diagram and the Bethe-Ansatz solution of the *six-vertex model for periodic and anti-periodic boundary conditions* are thoroughly discussed in the works of Lieb [17–20], Lieb, Wu [21], Sutherland [25], Baxter [3], Batchelor, Baxter,

O'Rourke, Yung [2]. See also the work of Wu, Lin [27], in which the Pfaffian solution for the six-vertex model with periodic boundary conditions is obtained on the free fermion line, $\Delta = 0$.

3 Izergin-Korepin Determinantal Formula

The *six-vertex model with DWBC* was introduced by Korepin in [14], who derived an important recursion relation for the partition function of the model. This lead to a beautiful *determinantal formula* of Izergin and Korepin [12], for the partition function of the six-vertex model with DWBC. A detailed proof of this formula and its generalizations are given in the paper of Izergin, Coker, and Korepin [13]. When the weights are parameterized according to (8), the formula of Izergin is

$$Z_N = \frac{[\sin(\gamma + t)\sin(\gamma - t)]^{N^2}}{(\prod_{n=0}^{N-1} n!)^2}\,\tau_N, \tag{9}$$

where τ_N is the Hankel determinant,

$$\tau_N = \det\left(\frac{d^{i+k-2}\phi}{dt^{i+k-2}}\right)_{1\le i,k\le N}, \tag{10}$$

and

$$\phi(t) = \frac{\sin(2\gamma)}{\sin(\gamma + t)\sin(\gamma - t)}. \tag{11}$$

An elegant derivation of the Izergin-Korepin determinantal formula from the *Yang-Baxter equations* is given in the papers of Korepin and Zinn-Justin [15] and Kuperberg [16].

One of the applications of the determinantal formula is that it implies that the partition function τ_N solves the *Toda equation*,

$$\tau_N \tau_N'' - {\tau_N'}^2 = \tau_{N+1}\tau_{N-1}, \quad N \ge 1, \ (') = \frac{\partial}{\partial t}, \tag{12}$$

cf. [24]. This was used by Korepin and Zinn-Justin [15] to derive the free energy of the six-vertex model with DWBC, assuming some Ansatz on the behavior of subdominant terms in the large N asymptotics of the free energy.

4 The Six-Vertex Model with DWBC and a Random Matrix Model

Another application of the Izergin-Korepin determinantal formula is that τ_N can be expressed in terms of a partition function of a *random matrix model*. The relation to

the random matrix model was obtained and used by Zinn-Justin [29]. This relation will be very important for us. It can be derived as follows. For the evaluation of the Hankel determinant, it is convenient to use the integral representation of $\phi(t)$, namely, to write it in the form of the Laplace transform,

$$\phi(t) = \int_{-\infty}^{\infty} e^{t\lambda} m(\lambda) d\lambda, \tag{13}$$

where

$$m(\lambda) = \frac{\sinh \frac{\lambda}{2}(\pi - 2\gamma)}{\sinh \frac{\lambda}{2}\pi}. \tag{14}$$

Then

$$\frac{d^i \phi}{dt^i} = \int_{-\infty}^{\infty} \lambda^i e^{t\lambda} m(\lambda) d\lambda, \tag{15}$$

and by substituting this into the Hankel determinant, (10), we obtain that

$$\begin{aligned} \tau_N &= \int \prod_{i=1}^{N} [e^{t\lambda_i} m(\lambda_i) d\lambda_i] \det(\lambda_i^{i+k-2})_{1\le i,k\le N} \\ &= \int \prod_{i=1}^{N} [e^{t\lambda_i} m(\lambda_i) d\lambda_i] \det(\lambda_i^{k-1})_{1\le i,k\le N} \prod_{i=1}^{N} \lambda_i^{i-1}. \end{aligned} \tag{16}$$

Consider any permutation $\sigma \in S_N$ of variables λ_i. From the last equation we have that

$$\tau_N = \int \prod_{i=1}^{N} [e^{t\lambda_i} m(\lambda_i) d\lambda_i] (-1)^{\sigma} \det(\lambda_i^{k-1})_{1\le i,k\le N} \prod_{i=1}^{N} \lambda_{\sigma(i)}^{i-1}. \tag{17}$$

By summing over $\sigma \in S_N$, we obtain that

$$\tau_N = \frac{1}{N!} \int \prod_{i=1}^{N} [e^{t\lambda_i} m(\lambda_i) d\lambda_i] \Delta(\lambda)^2, \tag{18}$$

where $\Delta(\lambda)$ is the Vandermonde determinant,

$$\Delta(\lambda) = \det(\lambda_i^{k-1})_{1\le i,k\le N} = \prod_{i<k} (\lambda_k - \lambda_i). \tag{19}$$

Equation (18) expresses τ_N in terms of a matrix model integral. Namely, if $m(x) = e^{-V(x)}$, then

$$\tau_N = \frac{\prod_{n=0}^{N-1} n!}{\pi^{N(N-1)/2}} \int dM e^{\mathrm{Tr}[tM - V(M)]}, \tag{20}$$

where the integration is over the space of $N \times N$ Hermitian matrices. The matrix model integral can be solved, furthermore, in terms of *orthogonal polynomials*.

Introduce monic polynomials $P_n(x) = x^n + \cdots$ orthogonal on the line with respect to the weight $w(x) = e^{tx}m(x)$, so that

$$\int_{-\infty}^{\infty} P_n(x)P_m(x)e^{tx}m(x)dx = h_n\delta_{nm}. \tag{21}$$

Then it follows from (18) that

$$\tau_N = \prod_{n=0}^{N-1} h_n. \tag{22}$$

The orthogonal polynomials satisfy the three term recurrence relation,

$$xP_n(x) = P_{n+1}(x) + Q_nP_n(x) + R_nP_{n-1}(x), \tag{23}$$

where R_n can be found as

$$R_n = \frac{h_n}{h_{n-1}}, \tag{24}$$

see, e.g., [26]. This gives that

$$h_n = h_0 \prod_{j=1}^{n} R_j, \tag{25}$$

where

$$h_0 = \int_{-\infty}^{\infty} e^{tx}m(x)dx = \frac{\sin(2\gamma)}{\sin(\gamma+t)\sin(\gamma-t)}. \tag{26}$$

By substituting (25) into (22), we obtain that

$$\tau_N = h_0^N \prod_{n=1}^{N-1} R_n^{N-n}. \tag{27}$$

5 Asymptotic Formula for the Recurrence Coefficients

We prove the following asymptotics of the recurrence coefficients R_n.

Theorem 1 (See [4]). *As $n \to \infty$,*

$$R_n = \frac{n^2}{\gamma^2}\left[R + \cos(n\omega)\sum_{j:\,\kappa_j\le 2} c_j n^{-\kappa_j} + cn^{-2} + O(n^{-2-\varepsilon})\right], \qquad \varepsilon > 0, \tag{28}$$

where the sum is finite and it goes over $j = 1, 2, \ldots$ such that $\kappa_j \le 2$,

$$R=\left(\frac{\pi}{2\cos\frac{\pi\zeta}{2}}\right)^2,\quad \zeta\equiv\frac{t}{\gamma};\qquad \omega=\pi(1+\zeta);\qquad \kappa_j=1+\frac{2j}{\frac{\pi}{2\gamma}-1},\tag{29}$$

and

$$c_j=\frac{2\gamma e^{\varphi(y_j)}}{\cos\frac{\pi\zeta}{2}}(-1)^j\sin\frac{\pi j}{1-\frac{2\gamma}{\pi}},\tag{30}$$

where

$$y_j=\frac{\pi j}{\frac{\pi}{2\gamma}-1},\tag{31}$$

and

$$\varphi(y)=-\frac{2y}{\pi}\ln\left(2\pi\cos\frac{\pi\zeta}{2}\right)+\frac{2}{\pi}\left[\int_0^\infty\arg(\mu+iy)f(\mu)d\mu+y\ln y-y\right],\tag{32}$$

where

$$f(\mu)=\frac{\pi}{2\gamma}\coth\mu\frac{\pi}{2\gamma}-\left(\frac{\pi}{2\gamma}-1\right)\coth\mu\left(\frac{\pi}{2\gamma}-1\right)-\operatorname{sgn}\mu.\tag{33}$$

Also,

$$c=\frac{\pi\gamma^2}{6(\pi-2\gamma)\cos^2\frac{\pi\zeta}{2}}-\frac{\pi^2}{48\cos^2\frac{\pi\zeta}{2}}.\tag{34}$$

The error term in (28) *is uniform on any compact subset of the set*

$$\left\{(t,\gamma):\ |t|<\gamma,\ 0<\gamma<\frac{\pi}{2}\right\}.\tag{35}$$

Remark. The method of the proof allows an extension of formula (28) to an asymptotic series in negative powers of n.

Denote

$$F_N=\frac{1}{N^2}\ln\frac{\tau_N}{(\prod_{n=0}^{N-1}n!)^2}.\tag{36}$$

From Theorem 1 we derive the following result.

Theorem 2. *As* $N\to\infty$,

$$F_N=F+O(N^{-1}),\tag{37}$$

where

$$F=\frac{1}{2}\ln\frac{R}{\gamma^2}=\ln\frac{\pi}{2\gamma\cos\frac{\pi\zeta}{2}}.\tag{38}$$

This coincides with the formula of work [29], obtained in the saddle-point approximation. Earlier it was derived in work [15], from some Ansatz for the free

energy asymptotics. For the partition function Z_N in (9) we obtain from Theorem 2 the formula,

$$\frac{1}{N^2}\ln Z_N = f + O(N^{-1}) \qquad f = \ln\left(\frac{\pi[\cos(2t) - \cos(2\gamma)]}{4\gamma\cos\frac{\pi t}{2\gamma}}\right). \tag{39}$$

Let us compare this formula and asymptotics (28) with known exact results.

6 Previous Exact Results

The free fermion line, $\gamma = \frac{\pi}{4}$, $|t| < \frac{\pi}{4}$. In this case the exact result is

$$Z_N = 1, \tag{40}$$

see, e.g., [9], which implies $f = 0$. This agrees with formula (39), which also gives $f = 0$ when $\gamma = \frac{\pi}{4}$. Moreover, the orthogonal polynomials in this case are the Meixner-Pollaczek polynomials, for which

$$R_n = \frac{4n^2}{\cos^2 2t} = \frac{n^2 R}{\gamma^2}, \tag{41}$$

cf. [9]. Thus, formula (28) is exact on the free fermion line, with no error term. This agrees with Theorem 1, because from (30), (34), $c_j = c = 0$ when $\gamma = \frac{\pi}{4}$.

The ASM (ice) point, $\gamma = \frac{\pi}{3}$, $t = 0$. In this case we obtain from (8) that

$$a = b = c = \frac{\sqrt{3}}{2}, \tag{42}$$

hence

$$Z_N = \left(\frac{\sqrt{3}}{2}\right)^{N^2} A(N), \tag{43}$$

where $A(N)$ is the number of configurations in the six-vertex model with DWBC. There is a one-to-one correspondence between the set of configurations in the six-vertex model with DWBC and the set of $N \times N$ alternating sign matrices. By definition, an alternating sign matrix (ASM) is a matrix with the following properties:

- All entries of the matrix are -1, 0, 1;
- If we look at the sequence of (-1)'s and 1's, they are alternating along any row and any column;
- The sum of entries is equal to 1 along any row and any column.

The above correspondence is established as follows: given a configuration of arrows on edges, we assign (-1) to any vertex of type (1) on Fig. 1, 1 to any vertex of type (2), and 0 to any vertex of other types. Then the configuration on the vertices gives

rise to an ASM, and this correspondence is one-to-one. For instance, Fig. 5 shows the ASM corresponding to the configuration of arrows on Fig. 2.

$$\begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & -1 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

Fig. 5 ASM for the configuration of Fig. 2

For the number of ASMs there is an exact formula:

$$A(N) = \prod_{n=0}^{N-1} \frac{(3n+1)!n!}{(2n)!(2n+1)!}. \tag{44}$$

This formula was conjectured in [22], [23], and proved by Zeilberger [28] by combinatorial arguments. Another proof was given by Kuperberg [16], who used formula (9). The relation to classical orthogonal polynomials was found by Colomo and Pronko [9], who used this relation to give a new proof of the ASM conjecture. The orthogonal polynomials in this case are the continuous Hahn polynomials and from [9] we find that

$$R_n = \frac{n^2(9n^2-1)}{4n^2-1} = \frac{9n^2}{4} + \frac{5}{16} + O(n^{-2}). \tag{45}$$

Formula (28) gives

$$R_n = \frac{9n^2}{\pi^2}\left[\frac{\pi^2}{4} + \frac{5\pi^2}{144n^2} + O(n^{-2-\varepsilon})\right], \tag{46}$$

which agrees with (45). From (44) we find that as $N \to \infty$,

$$A(N) = C\left(\frac{3\sqrt{3}}{4}\right)^{N^2} N^{-\frac{5}{36}}\left(1 - \frac{115}{15552N^2} + O(N^{-3})\right), \tag{47}$$

where $C > 0$ is a constant, so that

$$Z_N = C\left(\frac{9}{8}\right)^{N^2} N^{-\frac{5}{36}}\left(1 - \frac{115}{15552N^2} + O(N^{-3})\right), \quad N \to \infty. \tag{48}$$

Formula (39) gives $f = \ln\frac{9}{8}$, which agrees with the last formula.

The $x = 3$ ASM point, $\gamma = \frac{\pi}{6}$, $t = 0$. Here the exact result is

$$Z_N = \frac{3^{N/2}}{2^{N^2}} A(N; 3), \tag{49}$$

where

$$\begin{cases} A(2m+1;3) = 3^{m(m+1)} \prod_{k=1}^{m} [\frac{(3k-1)!}{(m+k)!}]^2, \\ A(2m+2;3) = 3^m \frac{(3m+2)!m!}{[(2m+1)!]^2} A(2m+1;3). \end{cases} \tag{50}$$

In this case $A(N;3)$ counts the number of alternating sign matrices with weight 3^k, where k is the number of (-1) entries. Formula (50) for $A(N;3)$ was conjectured in [22], [23] and proved in [16]. The relation to classical orthogonal polynomials was again found by Colomo and Pronko [9], who used it to give a new proof of formula (50) for the 3-enumeration of ASMs. The orthogonal polynomials in this case are expressed in terms of the continuous dual Hahn polynomials and from [9] we find that

$$R_{2m} = 36m^2, \qquad R_{2m+1} = 4(3m+1)(3m+2). \tag{51}$$

In this case the subdominant term in the asymptotics of R_n exhibits a period 2 oscillation. Namely, we obtain from the last formula that

$$R_n = 9n^2 + \frac{-1+(-1)^n}{2}. \tag{52}$$

This perfectly fits to the frequency value $\omega = \pi$ for $\zeta = 0$ in (29). Moreover, formula (28) gives

$$R_n = \frac{36n^2}{\pi^2}\left[\frac{\pi^2}{4} + \frac{(-1)^n c_1}{n^2} - \frac{\pi^2}{72n^2} + O(n^{-2-\varepsilon})\right], \tag{53}$$

which agrees with (52) and it provides with the value of $c_1 = \frac{\pi^2}{72}$.

From (50) we find, that as $m \to \infty$,

$$A(2m;3) = C_3 \left(\frac{3}{2}\right)^{4m^2} 3^{-m} (2m)^{\frac{1}{18}} \left(1 + \frac{77}{7776m^2} + O(N^{-3})\right), \tag{54}$$

where $C_3 > 0$ is a constant, and

$$A(2m+1;3) = C_3 \left(\frac{3}{2}\right)^{(2m+1)^2} 3^{-\frac{2m+1}{2}} (2m+1)^{\frac{1}{18}} \left(1 + \frac{131}{7776m^2} + O(m^{-3})\right). \tag{55}$$

so that

$$A(N;3) = C_3 \left(\frac{3}{2}\right)^{N^2} 3^{-\frac{N}{2}} N^{\frac{1}{18}} \left(1 + \frac{104 - 27(-1)^N}{1944N^2} + O(N^{-3})\right), \tag{56}$$

and

$$Z_N = C_3 \left(\frac{3}{4}\right)^{N^2} N^{\frac{1}{18}} \left(1 + \frac{104 - 27(-1)^N}{1944N^2} + O(N^{-3})\right), \quad N \to \infty. \tag{57}$$

Formula (39) gives $f = \ln \frac{3}{4}$, which agrees with the last formula.

We have the identity,

$$\frac{\partial^2 F_N}{\partial t^2} = \frac{R_N}{N^2}, \tag{58}$$

see, e.g., [5], which is equivalent to the Toda equation (12). By using identity (58), we obtain from Theorem 1 the following asymptotics.

Theorem 3. *As $N \to \infty$,*

$$\frac{\partial^2 (F_N - F)}{\partial t^2} = \frac{1}{\gamma^2} \cos(N\omega) \sum_{j:\, \kappa_j \le 2} c_j N^{-\kappa_j} + cN^{-2} + O(N^{-2-\varepsilon}). \tag{59}$$

This gives a quasiperiodic asymptotics, as $N \to \infty$, of the second derivative of the subdominant terms.

7 Zinn-Justin's Conjecture

Paul Zinn-Justin conjectured in [29] that

$$Z_N \sim C N^{\kappa} e^{N^2 f}, \tag{60}$$

i.e.,

$$\lim_{N\to\infty} \frac{Z_N}{C N^{\kappa} e^{N^2 f}} = 1. \tag{61}$$

Formulae (40), (48), and (57) confirm this conjecture, with the value of κ given as

$$\kappa = \begin{cases} 0, & \gamma = \frac{\pi}{4}, \quad |t| < \frac{\pi}{4}; \\ -\frac{5}{36}, & \gamma = \frac{\pi}{3}, \quad t = 0; \\ \frac{1}{18}, & \gamma = \frac{\pi}{6}, \quad t = 0. \end{cases} \tag{62}$$

Bogoliubov, Kitaev and Zvonarev obtained in [8] the asymptotics of Z_N on the line $\frac{a}{c} + \frac{b}{c} = 1$, separating the disordered and antiferroelectric phases. This corresponds to the value $\gamma = 0$. They found that in this case formula (60) holds with $\kappa = \frac{1}{12}$.

With the help of Theorem 1 we prove the following result.

Theorem 4. *We have that*

$$Z_N = C N^{\kappa} e^{N^2 f} \left(1 + O(N^{-\varepsilon})\right), \quad \varepsilon > 0, \tag{63}$$

where

$$\kappa = \frac{1}{12} - \frac{2\gamma^2}{3\pi(\pi - 2\gamma)}, \tag{64}$$

and $C > 0$ is a constant.

This proves the conjecture of Zinn-Justin, and it gives the exact value of the exponent κ. Let us remark, that the presence of the power-like factor N^{κ} in the asymptotic expansion of Z_N in (63) is rather unusual from the point of view of random matrix models. In the one-cut case the usual large N asymptotics of Z_N in a non-critical random matrix model is the so called "topological expansion", which gives Z_N as an asymptotic series in powers of $1/N^2$. For a rigorous proof of the "topological expansion" see the work of Ercolani and McLaughlin [10] (see also [5]).

8 Large N Asymptotics of Z_N in the Ferroelectric Phase

Recently Bleher and Liechty [7], [6] obtained the large N asymptotics of Z_N in the ferroelectric phase, $\Delta > 1$, and also on the critical line between the ferroelectric and disordered phases, $\Delta = 1$. In the ferroelectric phase we use parameterization (6) for a, b and c. The large N asymptotics of Z_N in the ferroelectric phase is given by the following theorem:

Theorem 5. *In the ferroelectric phase with $t > \gamma > 0$, for any $\varepsilon > 0$, as $N \to \infty$,*

$$Z_N = CG^N F^{N^2}\left[1 + O\left(e^{-N^{1-\varepsilon}}\right)\right], \tag{65}$$

where $C = 1 - e^{-4\gamma}$, $G = e^{\gamma - t}$, and $F = \sinh(t + \gamma)$.

On the critical line between the ferroelectric and disordered phases we use the parameterization $b = a + 1$, $c = 1$. The main result here is the following asymptotic formula for Z_N:

Theorem 6. *As $n \to \infty$,*

$$Z_N = CN^{\kappa} G^{\sqrt{N}} F^{N^2}[1 + O(N^{-1/2})], \tag{66}$$

where $C > 0$,

$$\kappa = \frac{1}{4}, \qquad G = \exp\left[-\zeta\left(\frac{3}{2}\right)\sqrt{\frac{a}{\pi}}\right], \tag{67}$$

and

$$F = b. \tag{68}$$

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Mathematical Issues in Loop Quantum Cosmology

Martin Bojowald

Abstract Focusing on mathematical aspects, this article gives a review of loop quantum cosmology as an application of background independent quantization techniques to cosmological models. Mathematical issues arise at two different levels. First, the kinematical basis of loop quantum cosmology is derived as an induced representation of loop quantum gravity. The discrete spatial geometry exhibited by quantum gravity as a consequence of the loop quantization is then realized also in cosmological models. Dynamical equations formulated in such models are difference rather than differential equations, whose analysis provides the second class of mathematical applications. Suitable solutions display typical features in quantum regimes, where they can resolve classical space-time singularities, but should also approach semiclassical behavior in classical regimes. Such solutions can be found using generating function or continued fraction techniques. Semiclassical behavior and corrections to the classical one are derived using effective equations which approximate partial difference equations by ordinary differential equations.

1 Introduction

In classical gravity, space-time is described as a solution of Einstein's equation $G_{ab} = 8\pi G T_{ab}$, relating the Einstein tensor $G_{ab} = R_{ab} - \frac{1}{2}Rg_{ab}$ of a space-time metric g_{ab} to the energy-momentum tensor T_{ab} of matter, with a coupling constant given by the gravitational constant G. Due to the Ricci tensor R_{ab}, this is a set of coupled non-linear partial differential equations for the metric with space-time coordinates as independent variables. These equations are difficult to solve, but

Martin Bojowald
Institute for Gravitational Physics and Geometry, The Pennsylvania State University, 104 Davey Lab, University Park, PA 16802, USA, e-mail: bojowald@gravity.psu.edu

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with some assumptions it is possible to derive general properties. One of the best known theorems states that for matter satisfying positive energy conditions, space-time solutions are generically geodesically incomplete: There is always a geodesic which is incomplete and cannot be extended beyond its defined range [34]. Such space-times are called singular due to the presence of boundaries to the motion of freely falling observers. In the best-known examples such as the Friedmann–Robertson–Walker or Schwarzschild solutions, some curvature scalars diverge at such boundaries, although this is not a general property proved in singularity theorems.

Canonical quantum gravity describes space-time by different structures, the metric no longer being the basic object. This requires a different mathematical formulation and poses new problems. A classical state is given by a point in phase space which for gravity is the cotangent bundle of the space of spatial metrics. Momenta, i.e. coordinates along the fibers, are given by the extrinsic curvature tensor of spatial slices Σ, which describes how the slice bends in space-time. A map from space-time metrics on a 4-dimensional manifold M as solutions to general relativity to points in this phase space is not given canonically but requires a choice of slicing $\Sigma_t : t = \text{const}$, given by a global time function $t : M \to \mathbb{R}$. Space-time geometries are independent of the time function chosen provided that the cotangent bundle of spatial metrics with its canonical symplectic form is symplectically reduced to the appropriate physical phase space. This is achieved by imposing constraints $C_i = 0$, $i = 1, \ldots, 4$ on the phase space variables which are equivalent to Einstein's equation.

In quantum gravity, analogously to quantum mechanics, a state is described by a vector in a (projective) Hilbert space. The Hilbert space is a representation space of the classical Lie algebra of basic variables, such as spatial metrics and extrinsic curvature, under taking Poisson brackets. Alternatively, states can be defined as positive linear functionals (expectation values) on the algebra itself. Such states can usually be represented as wave functionals on the configuration space, such as the space of spatial metrics or related objects for gravity. In analogy to the classical symplectic reduction, the Hilbert space with its representation of basic operators must be reduced by imposing constraints. These are obtained by representing the classical constraints as operators and asking that they annihilate physical states: $\hat{C}_i|\psi\rangle = 0$. This implies linear functional differential equations (in a Wheeler–DeWitt quantization [31, 46]) or functional difference equations (in loop quantum gravity [43, 3, 45]) where independent variables of the functional equations are the metric tensors. Issues specific to applications of those equations to quantum cosmology are described in [15].

In general, such operators are difficult to formulate, and the resulting equations difficult to solve. As in the classical theory, one often uses simplifications due to spatial symmetries such as homogeneity and isotropy in cosmological situations. This article describes the derivation of such reduced models as well as aspects of solutions to their quantum constraint equations.

2 Quantum Representation and Dynamical Equations

A classical symmetry reduction simply selects a subspace $\mathscr{P}_{\rm symm}$ of the full phase space $\mathscr{P}$, motivated by symmetry assumptions on metric and extrinsic curvature, for which the pull-back of the full symplectic structure Ω is also symplectic. The model thus inherits a well-defined phase space of its own, which allows one to define its dynamics by pulling back the full constraints C_i, defining the reduced constrained system.

2.1 Quantum Reduction

At the quantum level, one starts with a representation of basic operators on a Hilbert space on which symmetries are to be implemented. Since a classical symmetry condition has to be imposed on both configuration variables and momenta to ensure a symplectic reduced phase space, operators for those conjugate variables do not commute. One thus cannot impose symmetry conditions strongly as operator equations for states. A suitable formulation has been achieved by imposing symmetry conditions based on the consideration of appropriate states as well as operators [19]. Just as the full classical phase space induces a unique reduced phase space once the symmetry has been specified, the full basic quantum algebra, representing the classical configuration and momentum variables as operators, induces a unique reduced representation once the symmetry has been specified. For explicit constructions see [24, 11]. (The procedure is related to Rieffel induction [40, 39]. An alternative procedure, which does not fully remove non-symmetric degrees of freedom but requires that they are unexcited, is described in [32, 33]. At least for free quantum field theories this can be achieved using the usual coherent states.)

Given a Hilbert space representation, a symmetric state is defined as a distributional state in the full Hilbert space which is supported only on invariant configuration variables [19]. Here, one can take advantage of the fact that canonical general relativity can be formulated in terms of connections as configuration variables [1, 7], and of the classification of invariant connections on symmetric principal fiber bundles [38, 26]. Symmetry conditions for momenta are then imposed by the induced algebra: it is generated by all basic operators of the full theory which map the space of symmetric states into itself.

A simple example illustrates the procedure: Given $n+1$ degrees of freedom (q_i, p_i) from which the $(n+1)$st one is to be removed by symmetry reduction, we have to impose $q_{n+1} = 0 = p_{n+1}$. While this is straightforward classically, strong operator conditions $\hat{q}_{n+1}|\psi\rangle = 0 = \hat{p}_{n+1}|\psi\rangle$ in quantum mechanics would be inconsistent due to $0 = [\hat{q}_{n+1}, \hat{p}_{n+1}]|\psi\rangle = i\hbar|\psi\rangle$. Instead, one can perform the reduction as follows. Define a symmetric state to be a distribution $\Psi(q_i) = \delta(q_{n+1})\psi(q_i)$ in the dual $\mathscr{D}^*$ of a suitable dense subset $\mathscr{D}$ of the Hilbert space. This defines the set of symmetric states $\mathscr{D}_{\rm symm} \subset \mathscr{D}^*$. Any operator $\hat{O}$ which is well-defined on $\mathscr{D}$ has

a dual action on Ψ defined by $(\hat{O}\Psi)[\phi] = \Psi[\hat{O}^\dagger\phi]$ for all $\phi \in \mathscr{D}$. In particular the basic operators $(\hat{q}_i, \hat{p}_i)$ thus obtain a dual action on $\mathscr{D}^*$, but not all of them fix the subset $\mathscr{D}_{\rm symm}$. The induced algebra of the reduction is now defined as the algebra generated by the basic operators mapping $\mathscr{D}_{\rm symm}$ into itself, and their induced representation is obtained from the dual action. This leaves us with the correct degrees of freedom: $(\hat{q}_i, \hat{p}_i)$, $i = 1, \ldots, n$ satisfy the condition and are thus generators of the induced algebra. The derivative operator $\hat{p}_{n+1}$, however, does not fix $\mathscr{D}_{\rm symm}$ and is thus not part of the induced algebra, while $\hat{q}_{n+1}$ becomes the zero operator in the dual action. We thus have successfully derived the reduced algebra and an induced representation. Since the dual $\mathscr{D}^*$ does not carry a natural inner product related to that of the Hilbert space, there is initially no inner product on $\mathscr{D}_{\rm symm}$, either. The induced representation nevertheless carries a natural inner product defined by requiring the correct adjointness properties of generators of the induced algebra. In our example, $(\hat{q}_i, \hat{p}_i)$ have to be self-adjoint, such that the induced representation fully agrees with the usual quantum representation of the classically reduced system. Note that there is a difference to the classical situation: classical symmetric solutions are exact solutions of the general equations while the induced representation space, in general, is not a subspace of the full representation space. This arises because for the quantum theory it is not the representation space but the algebra of basic operators which is primary.

This procedure is general enough to apply to loop quantum gravity, too. It defines the symmetric sector of the full theory, derived from the full quantum representation. Already the derivation of the induced basic representation is crucial since the Stone–von Neumann theorem does not apply in loop quantum cosmology (holonomies not being weakly continuous in a loop quantization). Thus, there is no unique representation even in finite-dimensional systems and physical properties can be representation dependent. It is thus crucial that the representation of loop quantum cosmology is derived from that of full loop quantum gravity along the lines sketched above. This is the underlying reason for the availability of qualitative physical predictions.

2.2 Dynamics

On the induced representation one then has to formulate the constraints $\hat{C}_i$ and solve the equations they imply for states. The quantum analog of pulling back the classical constraints is not simple, unless they are linear in basic variables, and is still being developed. Rather than deriving quantum constraints in this way, one currently quantizes the reduced constraints from induced basic operators along the lines followed in a full construction. Since the most important aspects of quantum constraints and their solutions depend on the representation in which the operators are formulated, properties of constraints in the full theory are thus inherited in models through the induction procedure. This suffices to show crucial effects which enter the general quantization scheme, and has by now led to many applications. But, at a detailed level, it leaves several different possibilities for the exact form of

constraints, a degree of non-uniqueness which is exacerbated by the current non-uniqueness of the full constraint in the first place.

In most models introduced so far, the constraints take the form of difference equations for states. Once a model has been specified, loop quantum cosmology thus requires one to solve difference equations for a wave function. This leads to our second mathematical issue, properties of difference equations of a certain type. We will focus here on isotropic models, whose induced representation is given by the space of square integrable functions on the Bohr compactification of the real line [5, 14]. By this compactification, the representation differs from what one would expect naively from a quantum mechanical procedure as it is followed in Wheeler–DeWitt quantizations. This is an example for the importance of the induction procedure to impose symmetry conditions. As a direct implication, the momentum operator of isotropic models, corresponding to a densitized triad component and thus describing spatial geometry, has a discrete spectrum of eigenvalues μ. (Any real value of μ is allowed, but all eigenstates are normalizable: the Hilbert space is non-separable.) This is not only the reason for the occurrence of difference equations but also has further physical implications.

Only one constraint remains to be imposed in an isotropic model due to the symmetry. A corresponding operator has to be constructed in terms of the basic ones, following the steps one would do without assuming symmetries. This is indeed possible, but not in a unique manner. The resulting equation for a wave function ψ_μ is in general of the form of a difference equation [9]

$$\begin{aligned}(V_{\mu+2} - V_\mu)\psi_{\mu+1}(\phi) - 2(V_{\mu+1} - V_{\mu-1})\psi_\mu(\phi)\\ + (V_\mu - V_{\mu-2})\psi_{\mu-1}(\phi) = -\frac{4\pi G}{3}\hat{H}_{\text{matter}}(\mu)\psi_\mu(\phi)\end{aligned} \tag{1}$$

where coefficients are written in terms of volume eigenvalues $V_\mu = (|\mu|/6)^{3/2}$ and $\hat{H}_{\text{matter}}$ is a differential operator (quantizing the matter Hamiltonian) acting on the matter field ϕ.

This equation, as written here, is the simplest version, based on certain assumptions on how a full constraint operator would reduce to that of the model. The freedom one has in the full construction essentially reduces, in isotropic models, to the form of the step size of the dynamical difference equation. This can be phrased as the question of which function of μ, if any at all, changes equidistantly in the equation, which need not be the eigenvalue μ of the basic triad operator. A more general class can be formulated after replacing according to the canonical transformation $(c, p) \mapsto (p^k c, p^{1-k}/(1-k))$ which can be motivated by lattice refinements occurring in an inhomogeneous state and restricts k to the range $-1/2 < k < 0$ [14]. Then, μ^{1-k} instead of μ will be equidistant. So far, only the extreme cases $k = 0$ (with constant step size μ_0 in μ [5]) and $k = -1/2$ (with step size $\bar{\mu}(\mu) \propto 1/\sqrt{|\mu|}$ [6]) have been considered in some detail.

Fully realistic cases are somewhere in between with a μ-dependence which can only be determined from a precise relation to full dynamics. The general statements and techniques described in what follows are insensitive to the precise behavior or

the value of k. Coefficients of the difference equation, and also asymptotic properties, do however depend on the choice. Detailed investigations are now emerging which can shed light on more precise features of the difference equation and fix some of the freedom in their derivation. In general, one may have to consider non-equidistant difference equations, especially for less symmetric models where a partial difference equation results from anisotropy [10, 23] or even several coupled equations in inhomogeneous situations [22].

3 Quantum Singularity Problem

The first general property of difference equations of loop quantum cosmology which has been studied deals with the singularity problem [8]. In this context, the singularity problem arises as the question of whether or not wave functions solving the functional equations are uniquely extended across classical singularities on the configuration spaces of metrics or related objects [18]. As before, wave functions of loop quantum cosmology are first defined on the whole real axis $\mu \in \mathbb{R}$, which includes the classical singularity $\mu = 0$ as an interior point. Unlike for the Wheeler–DeWitt equation, solutions to the difference equation then extend uniquely from positive μ to negative μ and vice versa, even though coefficients of the difference equation may vanish. There is thus a well-posed initial value problem even across the classical singularity, which makes the quantum evolution non-singular. (The recurrence determined by the difference equation is not guaranteed to extend a wave function in such a way just by the fact that $\mu = 0$ is an interior point. The lowest order coefficient $V_\mu - V_{\mu-2}$ of $\psi_{\mu-1}$ vanishes at $\mu = 1$, and the backward evolution will thus not determine the value ψ_0 right at the classical singularity. If this value is needed for the further recurrence, additional input would be required and one would be dealing with a boundary value rather than initial value problem. Physically, the behavior of solutions would not be determined by values of the wave function at one side of the classical singularity only.) This extendability, called quantum hyperbolicity for the functional equations, replaces geodesic completeness as the criterion for non-singular behavior. Using symmetry reduction as described above, it is currently verified in many cases based on the difference equations of loop quantum cosmology [13], including inhomogeneous ones [8, 10, 23, 12]. This covers the quantum analogs of the basic classical examples of singular space-times.

In addition to the hyperbolicity issue, which can be rather involved especially in inhomogeneous models with coupled partial difference equations, the analysis of extendability leads to a further class of mathematical issues: To analyze the extendability of solutions across classical singularities in spaces of triads, one needs a characterization of classical singularities by geometrical properties. This is difficult in general as the singularity theorems do not provide much information on the behavior of the singularities they predict. Here, further simplifications occur in symmetric models where classical singularities can often be analyzed completely.

As one of the results, it turned out that the extendability of wave functions hinges on the type of variables used. Densitized triads E^a_i, related to the spatial metric by $E^a_i E^b_i = q^{ab} \det(q_{cd})$, are used as basic variables in loop quantum gravity. They naturally arise in setting up a background independent quantization and have, independently, led to a resolution of singularities in all cases studied so far. On the other hand, the spatial metric or even triads or co-triads, rather than densitized triads, do not provide a general mechanism. While any choice of triad variables offers an extended configuration space due to the sign provided by the triad orientation, the position of classical singularities in superspaces depends sensitively on the type of variables. In isotropic models the difference is not crucial, as demonstrated by the analysis of [36] following [5], but it is essential in anisotropic models as seen by comparing [41] with [2]. This is a consequence of the fact that anisotropic models, which unlike isotropic ones are often expected to show the typical approach to a space-like singularity, have finite densitized triad component but one infinite metric or co-triad component at the singularity. One can see this easily in the Kasner solution with metric components $a_I(t) \propto t^{\alpha_I}$ and densitized triad components $p^I(t) \propto t^{1-\alpha_I}$. Since the Kasner solution requires $\sum_I \alpha_I = 1 = \sum_I \alpha_I^2$ and thus $-1 < \alpha_I \leq 1$ with one coefficient always being negative, one a_I diverges while the p^I all approach zero at the classical singularity $t = 0$. A further analysis of more general singularities from this perspective can provide important insights for quantum gravity by a combination of mathematical relativity and properties of difference equations, linked by quantum dynamics.

4 Examples for Properties of Solutions

In addition to the singularity issue, questions about solutions to difference equations one is interested in are:

1. Is it possible to find exact special solutions to the difference equations of loop quantum cosmology in some cases? This is not easy in general, although we have a linear difference equation, due to the presence of non-constant coefficients involving an absolute value.
2. If no exact solution is known, what are asymptotic properties (for large $|\mu|$) of general solutions? This is often relevant for a normalization of wave functions in a physical inner product. There are two types of asymptotic behavior which are being investigated:
   (a) Oscillations on small scales (such as $\psi_\mu \sim (-1)^\mu$), which can often be analyzed by generating functions [29] and
   (b) Boundedness of solutions, where continued fractions can advantageously be applied [20].

   Let us first look at the difference equation

$$a_{m+1} - a_{m-1} = 2\lambda m^{-1} a_m$$

which arises when the partial difference equation of an anisotropic quantum cosmological model is separated [10, 29]. Here, $\lambda \in \mathbb{R}$ is the separation parameter. Solutions to this difference equation have generating function

$$G(x) = \sum_{m=0}^{\infty} a_{m+1} x^m = c_0(1+x)^{\lambda-1}(1-x)^{-\lambda-1} - \frac{2^\lambda a_0}{\lambda-1}(1-x)^{-\lambda-1}{}_2F_1(1-\lambda,-\lambda;2-\lambda;(1+x)/2)$$

which can advantageously be used to determine asymptotic properties. For instance, solutions have $(-1)^m$-oscillations with shrinking amplitude if $G(x)$ is regular at $x=-1$ because $\sum_m (-1)^m a_m$ must then be convergent. This requires special initial values of the solution satisfying

$$a_1/a_0 = 1 - \lambda\psi(1/2 - \lambda/2) + \lambda\psi(1-\lambda/2)$$

with the digamma function $\psi(z) = \mathrm{d}\log\Gamma(z)/\mathrm{d}z$. Moreover, the parameter c_0 in the generating function must vanish in this case. The initial values are determined through $a_1 = G(0)$ while a_0 already appears as a parameter in the generating function. Further applications of generating functions in this context can be found in [27, 30, 28].

Another difference equation is

$$s_{n+4} - 2s_n + s_{n-4} = \Lambda n s_n$$

which appears in isotropic models of Euclidean gravity including a cosmological constant Λ (see also [42] for an analysis of this model). Generic solutions to this equation exponentially increase for large n, but it is often important to determine special solutions which are bounded (and thus normalizable as states in an ℓ^2 Hilbert space). This also poses conditions on initial values of the solution, such that they equal the continued fraction [20]

$$\frac{s_0}{s_4} = 2 - \frac{1}{2+4\Lambda - \frac{1}{2+8\Lambda-\cdots}}. \tag{2}$$

Such results are true for more general difference equations than that shown above, but the one used here provides an interesting relation to Bessel functions. In fact, the displayed difference equation can be solved exactly in terms of Bessel functions,

$$s_n = C_1 J_{\frac{n}{4}+\frac{1}{2\Lambda}}\left(\frac{1}{2\Lambda}\right) + C_2 Y_{\frac{n}{4}+\frac{1}{2\Lambda}}\left(\frac{1}{2\Lambda}\right). \tag{3}$$

Only the first contribution is bounded which, by comparison with (2) and its analog for $s_{4(m_0-1)}/s_{4m_0}$ with integer m_0, gives the continued fraction representation

$$\frac{J_{m_0-1+\frac{1}{2\Lambda}}(\frac{1}{2\Lambda})}{J_{m_0+\frac{1}{2\Lambda}}(\frac{1}{2\Lambda})} = 2 + 4\Lambda m_0 - \cfrac{1}{2 + 4\Lambda(m_0+1) - \cfrac{1}{2+4\Lambda(m_0+2)-\cdots}}.$$

5 Effective Theory

Usually, for physical applications one is not primarily interested in solutions to difference equations, i.e. quantum states, but in the resulting expectation values and fluctuations of certain operators. These can then be directly compared with potential observations. There is a powerful method to compute such expectation values, fluctuations and other quantities directly without taking the detour of wave functions: effective theory. When it is applicable and manageable for a given system, its physical properties can be studied much more directly.

One possibility to formulate effective equations uses a geometrical formulation of quantum mechanics [37, 35, 4]. The Hilbert space is interpreted as an infinite-dimensional phase space with symplectic form $\Omega(\cdot,\cdot) = \frac{1}{2\hbar}\mathrm{Im}\langle\cdot,\cdot\rangle_\psi$, whose points are states ψ. Variables on the phase space are the expectation value functions $q(\psi) = \langle\hat{q}\rangle_\psi$, $p(\psi) = \langle\hat{p}\rangle_\psi$ together with fluctuations and higher moments

$$G^{a,n}(\psi) := \langle((\hat{q} - \langle\hat{q}\rangle)^{n-a}(\hat{p} - \langle\hat{p}\rangle)^a)_{\mathrm{Weyl}}\rangle_\psi$$

for $2 \leq n \in \mathbb{N}$, $a = 0, \ldots, n$. The subscript "Weyl" indicates that, for $a \neq 0$ and $a \neq n$, the ordering of operators $\hat{q}$ and $\hat{p}$ is chosen totally symmetric. A state ψ in the Hilbert space is thus mapped to an infinite collection of numbers obtained by computing expectation values in this state. However, not any collection of numbers $G^{a,n}$ corresponds to a state in the Hilbert space (this is related to the Hamburger moment problem). The most important restriction is the uncertainty relation

$$G^{0,2}G^{2,2} - (G^{1,2})^2 \geq \hbar^2/4$$

which follows from the Schwarz inequality of the Hilbert space seen as a Kähler manifold.

Just as the dynamics of ψ is given by the Schrödinger equation $i\hbar\dot{\psi} = \hat{H}\psi$, the dynamics of the quantum variables is given by the flow along the Hamiltonian vector field X_{H_Q} generated by the quantum Hamiltonian $H_Q(\psi) = \langle\hat{H}\rangle_\psi$ as a function on the phase space. It usually couples all the quantum variables as, e.g., in

$$\begin{aligned} H_Q = {} & \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 q^2 + U(q) + \frac{1}{2}\hbar\omega(\tilde{G}^{0,2} + \tilde{G}^{2,2}) \\ & + \sum_{n>2}\frac{1}{n!}\left(\frac{\hbar}{m\omega}\right)^{n/2} U^{(n)}(q)\tilde{G}^{0,n} \end{aligned}$$

for an anharmonic oscillator with classical Hamiltonian $H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega^2 q^2 + U(q)$. (Using dimensionless $\tilde{G}^{a,n} = \hbar^{-n/2}(m\omega)^{n/2-a}G^{a,n}$.) This Hamiltonian generates equations of motion

$$\dot{q} = X_{H_Q} q = p/m$$

$$\dot{p} = X_{H_Q} p = -m\omega^2 q - U'(q) - \sum_n \frac{1}{n!}(m^{-1}\omega^{-1}\hbar)^{n/2} U^{(n+1)}(q) G^{0,n}$$

$$\begin{aligned}\dot{G}^{a,n} = X_{H_Q} G^{a,n} &= -a\omega G^{a-1,n} + (n-a)\omega G^{a+1,n} - \frac{aU''}{m\omega} G^{a-1,n} \\ &+ \frac{\sqrt{\hbar} a U'''(q)}{2(m\omega)^{\frac{3}{2}}} G^{a-1,n-1} G^{0,2} + \frac{\hbar a U''''(q)}{3!(m\omega)^2} G^{a-1,n-1} G^{0,3} \\ &- \frac{a}{2}\left(\frac{\sqrt{\hbar} U'''(q)}{(m\omega)^{\frac{3}{2}}} G^{a-1,n+1} + \frac{\hbar U''''(q)}{3(m\omega)^2} G^{a-1,n+2}\right) \\ &+ \frac{a(a-1)(a-2)}{24}\left(\frac{\sqrt{\hbar} U'''(q)}{(m\omega)^{\frac{3}{2}}} G^{a-3,n-3} + \frac{\hbar U''''(q)}{(m\omega)^2} G^{a-3,n-2}\right) + \cdots .\end{aligned}$$

These are infinitely many coupled ordinary differential equations for infinitely many variables, equivalent to the partial Schrödinger equation. This system is in general much more complicated to analyze in this form, but in an adiabatic approximation in the quantum variables one can decouple and solve the equations order by order, reproducing the low energy effective action as it is known in particle physics [21, 44]. The reformulation is thus valuable for semiclassical and perturbative aspects.

In general, the high coupling of the equations of motion is barely manageable. The main requirement for the applicability of effective theory in this form is then the availability of an exactly solvable system which one can use as zeroth order of a perturbation expansion. For the solvable model itself, the equations decouple, which can then be exploited in a perturbation analysis even in more complicated systems. For low energy effective actions as mentioned above, the solvable model is the harmonic oscillator or a free quantum field theory. Cosmological models are different, but also here a solvable model is available: a spatially flat isotropic model sourced by a free, massless scalar [16]. According to general relativity it is governed by the Friedmann equation $q^2\sqrt{p} = \frac{1}{2}p^{-3/2}p_\phi^2$. (The gravitational variables are extrinsic curvature $q = \dot{a}$ and the spatial volume $p^{3/2} = a^3$ in terms of the scale factor a.) Solving for the scalar momentum p_ϕ gives the Hamiltonian $p_\phi = H = qp$ (also known as the Berry–Keating–Connes Hamiltonian), interpreted as generating evolution in ϕ. Note that there are different sign choices possible in the solution p_ϕ; see [17] for more details.

A loop quantization leads to a Hamiltonian operator $\hat{H} = -\frac{1}{2}i(\hat{J} - \hat{J}^\dagger)$ with $\hat{J} = \widehat{pe^{iq}}$. Due to the exponential, this is a finite shift operator giving rise to a difference equation as mentioned before. The analysis of this section, motivated by effective theory, thus provides a further example for studying properties of solutions to a difference equation without actually solving the difference equation.

Our basic variables $(\hat{p}, \hat{J})$ are non-canonical, forming a (trivially) centrally extended $\mathrm{sl}(2,\mathbb{R})$ algebra

$$[\hat{p}, \hat{J}] = \hbar\hat{J}, \qquad [\hat{p}, \hat{J}^\dagger] = -\hbar\hat{J}^\dagger, \qquad [\hat{J}, \hat{J}^\dagger] = -2\hbar\hat{p} - \hbar^2.$$

Since the Hamiltonian $\hat{H}$ is a linear combination of generators of the algebra, the system is linear and provides an example for a solvable model. As one can see easily, only finitely many of the equations of motion for expectation values and quantum variables are coupled to each other.

The choice of variables requires one to use non-symmetric operators $\hat{J}$, such that not all the expectation values and quantum variables are real. Instead of simple reality conditions as in canonical real variables, we have to make sure that all variables respect the relation $\hat{J}\hat{J}^\dagger = \hat{p}^2$. Taking expectation values, this implies $|J|^2 - p^2 = c$ where c is determined in terms of quantum variables and turns out to be constant in time. Moreover, for semiclassical states c is of the order $\hbar$.

The quantum Hamiltonian $H_Q = -\frac{1}{2}i(J - \bar{J})$ generates equations of motion

$$\dot{p} = -\frac{1}{2}(J + \bar{J}), \qquad \dot{J} = -\frac{1}{2}(p + \hbar) = \dot{\bar{J}}$$

with the bouncing solution

$$p(\phi) = H\cosh(\phi - \delta) - \hbar, \qquad J(\phi) = -H(\sinh(\phi - \delta) + i)$$

satisfying the reality condition $J\bar{J} = p^2 + O(\hbar)$.

In addition to expectation values, also uncertainties are of interest to determine how semiclassically a state behaves. Equations of motion for fluctuations are also linear, as they follow from the Hamiltonian,

$$\dot{G}^{0,2} = -2G^{1,2}, \qquad \dot{G}^{2,2} = -2G^{1,2}$$
$$\dot{G}^{1,2} = -\frac{1}{2}G^{2,2} - \frac{3}{2}G^{0,2} - \frac{1}{2}(p^2 - J\bar{J} + \hbar p + \hbar^2/2)\,.$$

Their initial values are not arbitrary but must satisfy the uncertainty relation

$$G^{0,2}G^{2,2} - |G^{1,2}|^2 \geq \frac{\hbar^2}{4}|J|^2\,.$$

For $H \gg \hbar$, the solution is given by $(\Delta p)^2 = G^{0,2} \approx \hbar H\cosh(2(\phi - \delta))$ with a constant of integration δ which determines the difference of bounce times of expectation values and fluctuations. More details of fluctuations and dynamical coherent states of this system are derived in [17].

6 Summary

Loop quantum cosmology as an induced representation of loop quantum gravity describes quantum gravitational dynamics by difference equations, which allows a discussion of the singularity problem and provides a dynamical solution in many models. To understand properties of solutions, techniques such as generating functions or continued fractions are available for a direct analysis of difference equations. But especially in view of the more complicated extension to inhomogeneous models with many coupled difference equations, more tools are needed. Moreover, lattice effects of inhomogeneous states [14] can lead to difference equations with non-equidistant step size [25].

An effective treatment allows the computation of interesting properties of a solution, such as the peak position and spread of wave packets, without knowing the full solution. In this way one can extract physically interesting properties, analogously to "low energy" aspects in particle physics, without having to know explicit solutions for states.

These techniques are especially powerful in a solvable bounce model. This provides an intuitive bounce picture in special models, sourced by a free scalar, as exact effective systems. As a solvable system it provides the basis for a perturbation scheme to include matter interactions and inhomogeneities. Even physical inner product issues to properly normalize wave functions are addressable at the effective level through reality conditions. This gives hope that the notorious physical inner product problem can be dealt with in full quantum gravity, too.

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Boundary Effects on the Interface Dynamics for the Stochastic Allen–Cahn Equation

Lorenzo Bertini, Stella Brassesco and Paolo Buttà

Abstract We consider a stochastic perturbation of the Allen–Cahn equation in a bounded interval $[-a, b]$ with boundary conditions fixing the different phases at a and b. We investigate the asymptotic behavior of the front separating the two stable phases in the limit $\varepsilon \to 0$, when the intensity of the noise is $\sqrt{\varepsilon}$ and $a, b \to \infty$ with ε. In particular, we prove that it is possible to choose $a = a(\varepsilon)$ such that in a suitable time scaling limit, the front evolves according to a one-dimensional diffusion process with a nonlinear drift accounting for a "soft" repulsion from a. We finally show that a "hard" repulsion can be obtained by an extra diffusive scaling.

1 Introduction

The reaction-diffusion equation

$$\frac{\partial m}{\partial t} = \frac{1}{2}\frac{\partial^2 m}{\partial x^2} - V'(m), \tag{1}$$

for V a two well non-degenerate symmetric potential that attains its minimum at $\pm \mathtt{m}$ is a well studied equation that appears in different contexts to study the formation and evolution of interfaces for systems where two stable phases coexist. (See [1] for

Lorenzo Bertini
Dipartimento di Matematica, Università di Roma 'La Sapienza', P.le Aldo Moro 2, 00185 Rome, Italy, email: bertini@mat.uniroma1.it

Stella Brassesco
Departamento de Matemáticas, Instituto Venezolano de Investigaciones Científicas, Apartado Postal 20632, Caracas 1020-A, Venezuela, email: sbrasses@ivic.ve

Paolo Buttà
Dipartimento di Matematica, Università di Roma 'La Sapienza', P.le Aldo Moro 2, 00185 Rome, Italy, email: butta@mat.uniroma1.it

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an instance.) The two phases are identified with $+\mathtt{m}$ and $-\mathtt{m}$, and they are known to be stationary stable solutions of (1). There is also a family $\mathscr{M}$ of stationary solutions $\overline{m}_\zeta$ of (1) that interpolate between $-\mathtt{m}$ and $+\mathtt{m}$, that is, they satisfy $\frac{1}{2}\overline{m}_\zeta'' = V'(\overline{m}_\zeta)$ and $\overline{m}_\zeta(\pm\infty) = \pm\mathtt{m}$. We have that

$$\mathscr{M} = \{\overline{m}_\zeta : \zeta \in \mathbb{R}\} \tag{2}$$

where $\overline{m}_\zeta(x) = \overline{m}(x-\zeta)$, $\overline{m}(x)$ being the centered solution, that is, $\overline{m}(0) = 0$. The convergence of $\overline{m}_\zeta(x)$ to the value of the pure phases as $x \to \pm\infty$ is known to be exponentially fast (see [13]) so $\overline{m}_\zeta$ is thought to represent a diffuse interface located at ζ.

A natural problem is then to study the evolution of an initial datum belonging (or close) to $\mathscr{M}$ under the dynamics given by a stochastic perturbation of (1). It is the subject of a series of papers (see [6, 7, 9, 8, 15] for precise statements), where it is shown that, if a space-time white noise $W(dx, dt)$ of intensity $\sqrt{\epsilon}$ is added to (1), then the solution $m^{(\epsilon)}(x,t)$ of

$$\frac{\partial m}{\partial t} = \frac{1}{2}\frac{\partial^2 m}{\partial x^2} - V'(m) + \sqrt{\epsilon}W(dx, dt) \tag{3}$$

with initial datum $m(x,0) = \overline{m}_{x_0}(x)$, satisfies $m^{(\epsilon)}(x, t\epsilon^{-1}) \approx \overline{m}(x - x_0 - B(t))$ as $\epsilon \to 0$, where $B(t)$ is a Browian motion.

The previous result is proved in [9] in fact for the spatial variable $x \in [-a, b]$, with $a = \epsilon^{-\alpha}$ and $b = \epsilon^{-\beta}$ for $\alpha, \beta > 0$, and Neumann boundary conditions at the endpoints. In the time scaling ϵ^{-1}, the fluctuations introduced by the noise govern the evolution of the interface, and the scaling of the endpoints make them so distant that the effects of the boundary conditions are not present in the limiting behavior. Moreover, it follows from the analysis in [9] that this picture remains true if for instance $a = C\log\epsilon^{-1}$ for sufficiently large C.

On the other hand, from the results in [10] and [17] for the deterministic evolution given by (1) with Neumann boundary conditions on $a = c\log\epsilon^{-1}$ for sufficiently small c and $b = \epsilon^{-\gamma}$, a deterministic drift to the left becomes dominant in the time scaling ϵ^{-1}, and the $+\mathtt{m}$ phase takes over finally. This is a finite size effect, contrasting to the slow motion for the interface when far enough from the endpoints, reminiscent of the stability of $\mathscr{M}$ in the infinite volume situation. Recall that in a bounded interval, the pure phases are the unique global attractors.

We consider here the effect of non-homogeneous Dirichlet boundary conditions that fix the two different phases at the endpoints of $[-a, b]$ on the evolution of a front located initially at zero, under the dynamics given by (3). In this case, there is a unique stationary stable solution of (1) m^*, which is close to $\overline{m}_{\frac{b-a}{2}}$ as $a, b \to \infty$. In particular, initial data close to $\overline{m}_\zeta$ are attracted to this profile, and the evolution is known to occur along a set $\mathscr{M}_{a,b}$, which is close to $\mathscr{M}$ as $a, b \to \infty$.

When a space-time white noise of intensity $\sqrt{\epsilon}$ is added, we look at the evolution of the interface at a time scaling of order ϵ^{-1}, in the case $a = C_0\log(\epsilon^{-1})$ and

$b = \epsilon^{-\beta}$ for some $\beta > 0$, and let $\epsilon \to 0$. The reason for that particular ϵ dependence for the endpoints is to determine the effect of the boundary condition at a, ignoring the effect from the other endpoint b. We show that we can choose C_0 such that the limiting dynamics feels both the fluctuations produced by the noise and a deterministic drift repelling the motion from the left, which is interpreted as a soft wall effect. Under a further rescaling, we prove convergence to a Brownian motion reflected at the origin, which can be seen a hard wall.

2 Results and Strategy of Proofs

The above discussed results hold for a potential V having the stated properties, but in order to fix ideas and to be able to compute the exact coefficients in what follows, we choose

$$V(m) = \frac{1}{4}\big(m^2 - 1\big)^2,$$

which attains its minimum at ± 1 and yields $\overline{m}(x) = \tanh(x)$.

For each $\epsilon > 0$ we consider $m^{(\epsilon)}(x,t)$ the solution of (3) with boundary conditions $m^{(\epsilon)}(-a,t) = -1$ and $m^{(\epsilon)}(b,t) = 1$ and $W(dx,dt)$ a space-time white noise, that is, a centered Gaussian field with

$$E\big(W(dx,dt)W(dx',dt')\big) = \delta(x-x')\delta(t-t')$$

for δ a Dirac delta. The usual way to give a precise meaning to the above is to write down an integral equation corresponding to (3) in terms of a heat kernel, to observe that then each term makes sense and to prove that the integral equation admits a solution continuous in both variables with probability one. (See for instance [12].) This is called a mild solution, and to that one we refer in what follows. For f a continuous function defined in $[-a,b]$, we denote $\|f\|_\infty = \sup_{x\in[-a,b]} |f(x)|$. Also, let $\mathscr{F}_t$ the σ-algebra generated by $\{\int_0^{t'} \phi(x)W(dx,ds) : \phi \in L^2[-a,b], t' \le t\}$

The main results that we obtain are stated precisely in the next theorem.

Theorem 1. *Let*

$$a := \frac{1}{4}\log\epsilon^{-1}, \qquad b := \epsilon^{-\beta} \quad \textit{for some } \beta > 0, \qquad \lambda := \log\epsilon^{-1}, \tag{4}$$

and denote by $m^{(\epsilon)}(x,t)$ the solution of (3) with boundary conditions $m^{(\epsilon)}(-a,t) = -1$, $m^{(\epsilon)}(b,t) = 1$ and initial datum $m_0^{(\epsilon)} \in C([-a,b])$, such that for each $\eta > 0$ we have

$$\lim_{\epsilon\to 0} \epsilon^{-\frac{1}{2}+\eta}\big\|m_0^{(\epsilon)} - \overline{m}_0\big\|_\infty = 0. \tag{5}$$

Then:

(i) *There exists an $\mathscr{F}_t$-adapted real process X_ϵ such that, for each $\theta, \eta > 0$,*

$$\lim_{\epsilon\to 0}\mathbb{P}\Big(\sup_{t\in[0,\lambda\epsilon^{-1}\theta]}\big\|m^{(\epsilon)}(\cdot,t)-\overline{m}_{X_\epsilon(t)}(\cdot)\big\|_\infty>\epsilon^{\frac{1}{2}-\eta}\Big)=0; \tag{6}$$

(ii) *The real process* $Y_\epsilon(\tau):=X_\epsilon(\epsilon^{-1}\tau)$, $\tau\in\mathbb{R}_+$, *converges weakly in* $C(\mathbb{R}_+)$ *to the unique strong solution* Y *of the stochastic equation*

$$\begin{cases} dY(\tau)=12\exp\{-4Y(\tau)\}d\tau+dB(\tau),\\ Y(0)=0, \end{cases} \tag{7}$$

where B *is a Brownian motion with diffusion coefficient* $\frac{3}{4}$;

(iii) *The real process* $Z_\epsilon(\theta):=\lambda^{-1/2}X_\epsilon(\lambda\epsilon^{-1}\theta)$, $\theta\in\mathbb{R}_+$, *converges weakly in* $C(\mathbb{R}_+)$ *to a Brownian motion with diffusion coefficient* $\frac{3}{4}$ *reflected at zero.*

Outline of proof: A complete proof of this result and details concerning the analysis can be seen in [3].

Let us denote by $m(t)$ the solution of (3) with initial condition m_0 as in the statement of the theorem, dropping from the notation ϵ and the spatial variable, so m(t) is thought as a (random) element of $C[-a,b]$.

The linearization of (3) around $\overline{m}_z$ is

$$\begin{aligned}\frac{\partial}{\partial t}\big(m(t)-\overline{m}_z\big)&=\frac{1}{2}\frac{\partial^2}{\partial x^2}\big(m(t)-\overline{m}_z\big)-V''(\overline{m}_z)\big(m(t)-\overline{m}_z\big)\\&\quad-3\overline{m}_z\big(m(t)-\overline{m}_z\big)^2-\big(m(t)-\overline{m}_z\big)^3+\sqrt{\epsilon}W(dx,dt)\end{aligned}$$

and from that it is not difficult to see that $m(t)-\overline{m}_z$ satisfies the integral equation

$$\begin{aligned}m(t)-\overline{m}_z&=\varphi_z-g_t^{(z)}(\varphi_z)+g_t^{(z)}\big(m_0-\overline{m}_z\big)\\&\quad-\int_0^t ds\,g_{t-s}^{(z)}\big[3\overline{m}_z\big(m(s)-\overline{m}_z\big)^2+\big(m(s)-\overline{m}_z\big)^3\big]\\&\quad+\sqrt{\epsilon}\int_0^t g_{t-s}^{(z)}W(dx,ds),\end{aligned} \tag{8}$$

where $g_t^{(z)}=\exp(-tH^{(z)})$ for $H^{(z)}$ the operator defined for $C^2[-a,b]$ functions f that vanish at the endpoints of $[-a,b]$ as $H^{(z)}(f)=-\frac{1}{2}f''+V''(\overline{m}_z)$, and φ_z the solution to the linear equation with "compensating" non homogeneous boundary conditions, that is φ_z satisfies

$$\frac{1}{2}\varphi_z''(x)-V''\big(\overline{m}_z(x)\big)\varphi_z(x)=0\quad\varphi_z(-a)=-1-\overline{m}_z(-a)\quad\varphi_z(b)=1-\overline{m}_z(b)$$

It can be seen from the above equation that, for $\gamma>0$ small enough, given $\eta>0$

$$\lim_{\epsilon\to 0}\mathbb{P}\Big(\sup_{t\le\epsilon^{-\gamma}}\big\|m(t)-\overline{m}_0\big\|_\infty>\epsilon^{\frac{1}{2}-\eta}\Big)=0.$$

We would like to prove that the solution remains close to $\mathscr{M}$ for times of order of $\lambda\epsilon^{-1}$, and to identify $X_\epsilon(t)$ satisfying (6) and (iii), but this cannot be obtained directly from (8). The strategy we follow is to consider iterations of the linearization as described, over consecutive intervals of length $T = \epsilon^{-\gamma}$, updating at the beginning of the $k-th$ interval the location z_k of the interface $\overline{m}_{z_k}$ around which the linearization is performed. The z_k that showed to be convenient is the "center" of the solution $m(T_k)$, for $T_k = kT$, where the center $\zeta \in \mathbb{R}$ of a profile f in a neighborhood of $\mathscr{M}$ is the ζ such that

$$\langle f - \overline{m}_\zeta, \overline{m}'_\zeta \rangle := \int_{-a}^{b} dx (f - \overline{m}_\zeta)\overline{m}'_\zeta = 0.$$

Except for technicalities, the process $X_\epsilon(t)$ in the statement is given by the center of the solution $m(t)$. It is not difficult to obtain that the first order approximation (in terms of $\|f - \overline{m}_z\|_\infty$) for the center ζ of a given f is given by $\zeta - z \approx -\frac{3}{4}\langle \overline{m}'_z, f - \overline{m}_z \rangle$. In particular, applying the above procedure to $m(t)$ for $t \in [T_k, T_{k+1}]$ as explained we obtain, after projecting both sides of an equation analogous to (8), an approximation for the difference of the centers of the solution on that interval:

$$\begin{aligned} z_{k+1} - z_k &\approx -\frac{3}{4}\langle m(T_{k+1}) - \overline{m}'_{z_k}, \overline{m}'_{z_k} \rangle \\ &= -\frac{3}{4}\Bigg[\langle g_T^{(z_k)}(m(T_k) - \overline{m}_{z_k}), \overline{m}'_{z_k} \rangle + \langle \varphi_{z_k} - g_T^{(z_k)}(\varphi_{z_k}), \overline{m}'_{z_k} \rangle \\ &\quad + \left\langle \int_{T_k}^{T_{k+1}} ds\, g_{T_{k+1}-s}^{(z_k)}[NLT], \overline{m}'_{z_k} \right\rangle \\ &\quad + \sqrt{\epsilon}\left\langle \int_{T_k}^{T_{k+1}} g_{T_{k+1}-s}^{(z_k)} W(dx, ds), \overline{m}'_{z_k} \right\rangle \Bigg], \end{aligned} \tag{9}$$

where NLT are the non linear terms appearing between square brackets in (8).

The next step is to sum in k, for $k = 0, 1, \ldots, [t\epsilon^{-1+\gamma}]$, and to prove first that, as $\epsilon \to 0$, the z_k remain bounded, so basically (6) holds. Rough estimates follow from Gaussian estimates for the terms coming from the noise, conditioned on the value of the z_k, as for instance in [2].

Second, we show that what we obtain after taking $\epsilon \to 0$ is a discrete version of the integral equation for $Y(t)$. To give an idea of why this is true, let us analyze briefly the terms in (9). To really accomplish the program (including controlling the errors behind the symbol $\approx$) involves very precise estimates on the linear operators $H^{(z_k)}$ in finite intervals whose extremes depend on ϵ as described. See [11] and [20].

It can be seen that the first term in the second line does not contribute to the limit, from estimates on the spectral gap for $H^{(z_k)}$ uniform in ϵ and from the definition of center.

That the non linear terms also do not contribute follows from a precise analysis of the sum in k of the corresponding terms. For the last term in (8) we have that

$\langle g^{(z_k)}_{T_{k+1}-s} W(dx, ds), \overline{m}'_{z_k} \rangle \approx \sqrt{\frac{4}{3}} dB(s)$, so it will give the Brownian motion in the limiting equation. Finally, for the remaining term we have $-\frac{3}{4}\langle \varphi_{z_k} - g^{(z_k)}_T(\varphi_{z_k}), \overline{m}'_{z_k} \rangle \approx -\sqrt{\frac{3}{4}}\lambda_0 T \langle \varphi_{z_k}, \Psi_0 \rangle$, where λ_0 and Ψ_0 are the first eigenvalue and corresponding eigenvector of $H^{(z_k)}$. Since we can show $\lambda_0 \approx 24 \exp 4(a + z_k)$, after estimating Ψ_0 and computing φ_{z_k} it is possible to conclude that this term gives precisely the drift in (7).

Finally, to prove (iii), we show that the previous analysis can be extended for times of the order $\lambda\epsilon^{-1}$, and then, as the equation

$$dU_\lambda(t) = 12\lambda^{\frac{1}{2}} \exp\big(-4\lambda^{\frac{1}{2}} U_\lambda(t)\big)dt + W(t)$$

for $U_\lambda(t) := \lambda^{-\frac{1}{2}} Y(\lambda t)$, with W a Brownian motion with diffusion coefficient $\frac{3}{4}$ suggests, we obtain convergence to a reflected Brownian motion. (See [18] for basic concepts).

As a final comment, let us say that the analysis can be extended to the symmetric interval $[-a, b]$ with $a = b = \frac{1}{4}\log(\epsilon^{-1})$, obtaining for the corresponding process $Y(t)$ describing the motion of the interface the equation

$$dY(t) = 24 \sinh(4Y(t))dt + dB(t),$$

where it appears a wall effect from both sides.

The result is used in [4] to show convergence (as $\epsilon \to 0$) of the invariant measure for the solution of (3) with boundary conditions ± 1 in the symmetric interval to a nontrivial limit related to the invariant measure for the limiting process $Y(t)$.

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Dimensional Entropies and Semi-Uniform Hyperbolicity

Jérôme Buzzi

Abstract We describe *dimensional entropies* introduced in Buzzi (Bull. Soc. Math. France 126(1):51–77, 1998) list some of their properties, giving some proofs. These entropies allowed the definition in Buzzi (On entropy-expanding maps, preprint 2000; Cours de Saint-Flour, in preparation, 2009) of *entropy-expanding maps*. We introduce a new notion of *entropy-hyperbolicity* for diffeomorphisms. We indicate some simple sufficient conditions (some of them new) for these properties. We conclude by some work in progress and more questions.

1 Introduction

We are interested in using robust entropy conditions to study chaotic dynamical systems. These entropy conditions imply some "semi-uniform" hyperbolicity. This is a type of hyperbolicity which is definitely weaker than classical uniform hyperbolicity but which is stronger than Pesin hyperbolicity, that is, non vanishing of the Lyapunov exponents of some relevant measure. This type of conditions allows the generalization of some properties of interval maps and surface diffeomorphisms to arbitrary dimensions.

In this paper, we first explain what is known in low dimension just assuming the non-vanishing of the topological entropy $h_{\text{top}}(f)$. Then we give a detailed description of the *dimensional entropies*. These are $d+1$ numbers, if d is the dimension of the manifold,

$$0 = h^0_{\text{top}}(f) \leq h^1_{\text{top}}(f) \leq \cdots \leq h^d_{\text{top}}(f) = h_{\text{top}}(f).$$

Jérôme Buzzi
Laboratoire de Mathematique d'Orsay C.N.R.S., Université de Paris-Sud, Orsay Cedex, France, e-mail: jerome.buzzi@math.u-psud.fr

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$h^k_{\mathrm{top}}(f)$ "counts" the number of orbits starting from an arbitrary compact and smooth k-dimensional submanifold. We both recall known properties and establish new ones. We then recall the definition of *entropy-expanding maps* which generalize the complexity of interval dynamics with non-zero topological entropy. We also introduce a similar notion for diffeomorphisms:

Definition 1. A diffeomorphism of a d-dimensional manifold is *entropy-hyperbolic* if there are integers d_u, d_s such that:

- $h^{d_u}_{\mathrm{top}}(f) = h_{\mathrm{top}}(f)$ and this fails for every dimension $k < d_u$;
- $h^{d_s}_{\mathrm{top}}(f^{-1}) = h_{\mathrm{top}}(f)$ and this fails for every dimension $k < d_s$;
- $d_u + d_s = d$.

We give simple sufficient conditions for entropy – expansion and entropy – hyperbolicity. Finally we announce some work in progress and state a number of questions.

We now recall some classical notions which may be found in [20]. In this paper, all manifolds are compact.

A basic measure of orbit complexity of a map $f : M \to M$ is the *entropy*. The *topological entropy* $h_{\mathrm{top}}(f)$ "counts" all the orbits and the *measure-theoretic entropy* (also known as Kolmogorov-Sinai entropy or ergodic entropy) $h(f, \mu)$ "counts" the orbits "relevant" to some given invariant probability measure μ. They are related by the following rather general variational principle. If, e.g., f is continuous and M is compact, then

$$h_{\mathrm{top}}(f) = \sup_{\mu} h(f, \mu)$$

where μ ranges over all invariant probability measures. One can also restrict μ to *ergodic* invariant probability measures.

This brings to the fore measures which realize the above supremum, when they exist, and more generally measures which have entropy close to this supremum.

As $\mu \mapsto h(f, \mu)$ is affine, μ has maximum entropy if and only if almost every ergodic component of it has maximum entropy. Hence, with respect to entropy, it is enough to study ergodic measures.

Definition 2. A *maximum measure* is an ergodic and invariant probability measure μ such that $h(f, \mu) = \sup_\nu h(f, \nu)$.

A *large entropy measure* is an ergodic and invariant probability measure μ such that $h(f, \mu)$ is close to $\sup_\nu h(f, \nu)$.

The *Lyapunov exponents* for some ergodic and invariant probability measure μ are the possible values μ-a.e. of the limit $\lim_{n\to\infty} \frac{1}{n} \log \|T_x f^n . v\|$ where $\|\cdot\|$ is some Riemannian structure and $T_x f$ is the differential of f and v ranges over the non-zero vectors of the tangent space $T_x M$.

A basic result connecting entropy and hyperbolicity is the following theorem (proved by Margulis for volume preserving flows):

Theorem 3 (Ruelle's inequality). *Let $f : M \to M$ be a C^1 map on a compact manifold. Let μ be an f-invariant ergodic probability measure. Let $\lambda_1(\mu) \geq \cdots$ be its Lyapunov exponents repeated according to multiplicity. Then,*

$$h(f, \mu) \leq \sum_{i=1}^{d} \lambda_i(\mu)^+.$$

In good cases (with enough hyperbolicity), the entropy is also reflected in the existence of many periodic orbits:

Definition 4. The periodic points of some map $f : M \to M$ satisfy a *multiplicative lower bound*, if, for some integer $p \geq 1$:

$$\liminf_{n \to \infty, p|n} e^{-nh_{\text{top}}(f)} \#\{x \in [0, 1] : f^n x = x\} > 0.$$

Recall that many diffeomorphisms have infinitely many more periodic orbits (see [17, 18]).

The following type of isomorphism will be relevant to describe all "large entropy measures".

Definition 5. For a given measurable dynamical system $f : M \to M$, a subset $S \subset M$ is *entropy-negligible* if there exists $h < \sup_\mu h(f, \mu)$ such that for all ergodic and invariant probability measures μ with $h(f, \mu) > h$, $\mu(S) = 0$.

An *entropy-conjugacy* between two measurable dynamical systems $f : M \to M$ and $g : N \to N$ is a bi-measurable invertible mapping $\psi : M \setminus M_0 \to N \setminus N_0$ such that: ψ is a conjugacy (i.e., $g \circ \psi = \psi \circ f$) and M_0 and N_0 are entropy-negligible.

2 Low Dimension

Low dimension dynamical systems here means interval maps and surface diffeomorphisms—those systems for which non-zero entropy is enough to ensure hyperbolicity of the large entropy measures.

2.1 Interval Maps

Indeed, an immediate consequence of Ruelle's inequality on the interval is that a lower bound on the measure-theoretic entropy gives a lower bound on the (unique) Lyapunov exponent. Thus, invariant measures with nonzero topological entropy are hyperbolic in the sense of Pesin. One can obtain much more from the topological entropy:

Theorem 6. *Let $f : [0, 1] \to [0, 1]$ be C^∞. If $h_{\text{top}}(f) > 0$ then f has finitely many maximum measures. Also the periodic points satisfy a multiplicative lower bound.*

This was first proved by F. Hofbauer [15, 16] for piecewise monotone maps (admitting finitely many points $a_0 = 0 < a_1 < \cdots < a_N = 1$ such that $f|]a_i, a_{i+1}[$ is continuous and monotone). It was then extended to arbitrary C^∞ maps in [5]. In both settings, one builds an entropy-conjugacy to a combinatorial model called a Markov shift (which is a subshift of finite type over an infinite alphabet). One can then apply some results of D. Vere-Jones [26] and B. Gurevič [14].

We can even classify these dynamics. Recall that the *natural extension* of $f : M \to M$ is $\bar{f} : \bar{M} \to \bar{M}$ defined as $\bar{M} := \{(x_n)_{n\in\mathbb{Z}} \in M^{\mathbb{Z}} : \forall n \in \mathbb{Z}\ x_{n+1} = f(x_n)\}$ and $\bar{f}((x_n)_{n\in\mathbb{Z}}) = (f(x_n))_{n\in\mathbb{Z}}$. Recall that $\bar{\pi} : (x_n)_{n\in\mathbb{Z}} \mapsto x_0$ induces a homeomorphism between the spaces of invariant probability measures which respects entropy and ergodicity.

Theorem 7. *The natural extensions of C^∞ interval maps with non-zero topological entropy are classified up to entropy-conjugacy by their topological entropy and finitely many integers* (*which are "periods" of the maximum measures*).

The classification is deduced from the proof of the previous theorem by using a classification result [2] for the invertible Markov shifts involved.

The C^∞ is necessary: for each finite r, there are C^r interval maps with non-zero topological entropy having infinitely many maximum measures and others with none.

Remark 8. These examples show in particular that Pesin hyperbolicity of maximum measures or even of large entropy measures (which are both consequences of Ruelle's inequality here) are not enough to ensure the finite number of maximum measures.

2.2 Surface Transformations

As observed by Katok [19], Ruelle's inequality applied to a surface diffeomorphism and its inverse (which has opposite Lyapunov exponents) shows that a lower-bound on measure-theoretic entropy bounds away from zero the Lyapunov exponents of the measure. Thus, for surface diffeomorphisms also, nonzero entropy implies Pesin hyperbolicity.

It is believed that surface diffeomorphisms should behave as interval maps, leading to the following folklore conjecture:

Conjecture 9. Let $f : M \to M$ be a C^∞ surface diffeomorphism. If $h_{\text{top}}(f) > 0$ then f has finitely many maximum measures.

I would think that, again like for interval maps, finite smoothness is not enough for the above result. However counter-examples to this (or to existence) are known only in dimension ≥ 4 [22].

The best result for surface diffeomorphisms at this point is the following "approximation in entropy" [19]:

Theorem 10 (A. Katok). *Let $f : M \to M$ be a $C^{1+\epsilon}$ surface diffeomorphism. For any $\epsilon > 0$, there exists a horseshoe*[1] *$\Lambda \subset M$ such that $h_{\text{top}}(f|\Lambda) > h_{\text{top}}(f) - \epsilon$. In particular, the periodic points of f satisfy a logarithmic lower bound*:

$$\limsup_{n\to\infty} \frac{1}{n} \log \#\{x \in M : f^n(x) = x\} \geq h_{\text{top}}(f).$$

Katok in fact proved a more general fact, valid for any $C^{1+\epsilon}$-diffeomorphism of a compact manifold of any dimension. Namely, if μ is an ergodic invariant probability measure without zero Lyapunov exponent :

$$\limsup_{n\to\infty} \frac{1}{n} \log \#\{x \in M : f^n(x) = x\} \geq h(f, \mu).$$

On surfaces, Ruelle's inequality and the variational principle imply the theorem as explained above.

I have proved the conjecture for a model class, which replaces distortion with (simple) singularities [8]:

Theorem 11. *Let $f : M \to M$ be a piecewise affine homeomorphism. If $h_{\text{top}}(f) > 0$ then f has finitely many maximum measures.*

3 Dimensional Entropies

We are going to define the dimensional entropies for a smooth self-map or diffeomorphism $f : M \to M$ of a d-dimensional compact manifold. We will then investigate these quantities by considering other growth rates obtained from the volume and size of the derivatives.

3.1 Singular Disks

The basic object is:

Definition 12. A (*singular*) *k-disk* is a map $\phi : Q^k \to M$ with $Q^k := [-1, 1]^k$. It is C^r if it can be extended to a C^r map on a neighborhood of Q^k.

We need to define the C^r size $\|\phi\|_{C^r}$ of a singular disk ϕ for $1 \leq r \leq \infty$ as well as the corresponding topologies on the space of such disks. This involves some technicalities as vectors in different tangent spaces are not comparable *a priori*. We refer to Appendix 8 for the precise definitions, which are rather obvious for finite r. For $r = \infty$, we need an approximation property (which fails for some otherwise

[1] A horseshoe is an invariant compact subset on which some iterate of f is conjugate with a full shift on finitely many symbols.

very reasonable definitions of C^r size), Fact 57, which is used to prove Lemma 18 below.

From now on, we fix some C^r size arbitrarily on the manifold M. We will later check that the entropies we are interested in are in fact independent of this choice.

Notations. It will be convenient to sometimes write ϕ instead of $\phi(Q^k)$, e.g., $h_{\text{top}}(f, \phi)$ instead of $h_{\text{top}}(f, \phi(Q^k))$.

3.2 Entropy of Collections of Subsets

Given a collection $\mathscr{D}$ of subsets of M, we associate the following entropies. Recall that the (ϵ, n)-covering number of some subset $S \subset M$ is:

$$r_f(\epsilon, n, S) := \min\left\{\#C : \bigcup_{x\in S} B_f(\epsilon, n, x) \supset S\right\}$$

where $B_f(\epsilon, n, x) := \{y \in M : \forall 0 \leq k < n \ d(f^k y, f^k x) < \epsilon\}$ is the (ϵ, n)-dynamic ball. The classical Bowen-Dinaburg formula for the topological entropy of $S \subset M$ is $h_{\text{top}}(f, S) = \lim_{\epsilon\to 0} \limsup_{n\to\infty} \frac{1}{n} \log r_f(\epsilon, n, S)$ and $h_{\text{top}}(f) = h_{\text{top}}(f, M)$.

Definition 13. The *topological entropy* of $\mathscr{D}$ is:

$$h_{\text{top}}(f, \mathscr{D}) := \sup_{D\in\mathscr{D}} h_{\text{top}}(f, D) = \sup_{D\in\mathscr{D}} \lim_{\epsilon\to 0} \limsup_{n\to\infty} \frac{1}{n} \log r_f(\epsilon, n, D).$$

The *uniform topological entropy* of $\mathscr{D}$ is:

$$H_{\text{top}}(f, \mathscr{D}) := \lim_{\epsilon\to 0} \limsup_{n\to\infty} \frac{1}{n} \log \sup_{D\in\mathscr{D}} r_f(\epsilon, n, D).$$

Clearly $h_{\text{top}}(f, \mathscr{D}) \leq H_{\text{top}}(f, \mathscr{D})$. The inequality can be strict as shown in the following examples (the first one involving non-compactness, the second one involving non-smoothness).

Example 14. Let $T : \mathbb{T}^2 \to \mathbb{T}^2$ be a linear endomorphism with two eigenvalues Λ_1, Λ_2 with $1 < |\Lambda_1| < |\Lambda_2|$. Let $\mathscr{L}$ be the set of finite line segments. We have

$$0 < h_{\text{top}}(T, \mathscr{L}) = \log|\Lambda_2| < H_{\text{top}}(T, \mathscr{L}) = \log|\Lambda_1| + \log|\Lambda_2|.$$

Example 15. There exist a C^∞ self-map F of $[0, 1]^2$ and a collection $\mathscr{C}$ of C^r curves with bounded C^r norm such that $0 < h_{\text{top}}(F, \mathscr{C}) < H_{\text{top}}(F, \mathscr{C})$. This can be deduced from the example with $h^1_{\text{top}}(f \times g) > \max(h_{\text{top}}(f), h_{\text{top}}(g))$ in [6] by considering curves with finitely many bumps converging C^r to the example curve there, which has infinitely many bumps.

3.3 Definitions of the Dimensional Entropies

We can now properly define the dimensional entropies. Recall that we have endowed M with a C^r size.

Definition 16. For each $1 \leq r \leq \infty$, the *standard family* of C^r singular k-disks is the collection of all C^r singular k-disks. For finite r, the *standard uniform family* of C^r singular k-disks is the collection of all C^r singular k-disks with C^r size bounded by 1.

Definition 17. The C^r, *k-dimensional entropy* of a self-map f of a compact manifold is:

$$h_{\text{top}}^{k,C^r}(f) := h_{\text{top}}(f, \mathscr{D}_r^k)$$

where $\mathscr{D}_r^k$ is a standard family of C^r k-disks of M. We write $h_{\text{top}}^k(f)$ for $h^{k,C^\infty}(f)_{\text{top}}$ and call it the k-dimensional entropy.

The C^r, *k-dimensional uniform entropy* $H_{\text{top}}^{k,C^r}(f)$ is obtained by replacing $h_{\text{top}}(f, \mathscr{D}_r^k)$ with $H_{\text{top}}(f, D_r^k)$ in the above definition where D_r^k is the standard uniform family. We write $H_{\text{top}}^k(f)$ for $H_{\text{top}}^{k,C^\infty}(f)$ and call it the k-dimensional uniform entropy.

Observe that $h_{\text{top}}^{k,C^r}(f)$ and $H_{\text{top}}^{k,C^r}(f)$ are non-decreasing functions of k and non-increasing functions of r. Indeed, (1) $\mathscr{D}_r^k \supset \mathscr{D}_s^k$ and $D_r^k \supset D_s^k$ if $r \leq s$; (2) for any $0 \leq \ell \leq k \leq d$, restricting a k-disk to $[0,1]^\ell \times \{0\}^{k-\ell}$ does not increase its C^r size. Observe also that $h_{\text{top}}^{0,C^r}(f) = 0$ and $h_{\text{top}}^d(f) = h_{\text{top}}(f)$.

Lemma 18. *Let $f : M \to M$ be a C^∞ self-map of a compact manifold. We have*:

$$H_{\text{top}}^k(f) = \lim_{r \to \infty} H_{\text{top}}^{k,C^r}(f)$$

and the limit is non-increasing.

We shall see later in Proposition 38 that the same holds for $h_{\text{top}}^k(f)$.

Proof. We use one of the (simpler) ideas of Yomdin's theory. For each $n \geq 1$, we divide Q^k into small cubes with diameter at most $(\epsilon/4)^{1/r} \|\phi\|_{C^r}^{-1/r} \text{Lip}(f)^{-n/r}$. We need $(\epsilon/4)^{-k/r} \sqrt{k}^k \|\phi\|_{C^r}^{k/r} \text{Lip}(f)^{\frac{k}{r}n}$ such cubes. Let q be one of them. By Fact 57, there exists a C^∞ k-disk ϕ_q such that $\|\phi_q\|_{C^\infty} \leq 2\|\phi\|_{C^r}$ and

$$\begin{aligned} \forall t \in q \quad d(\phi_q(t), \phi(t)) &\leq \|\phi\|_{C^r} \|t - t_q\|^r \leq \|\phi\|_{C^r} \times \frac{\epsilon}{2} \|\phi\|_{C^r}^{-1} \text{Lip}(f)^{-n} \\ &\leq \frac{\epsilon}{2} \text{Lip}(f)^{-n}. \end{aligned}$$

It follows that $r_f(\epsilon, n, \phi \cap q) \leq r_f(\epsilon/2, n, \phi_q)$. Thus,

$$r_f(\epsilon, n, \mathscr{D}_r^k) \leq \sqrt{k}^k (\epsilon/4)^{-k/r} \|\phi\|_{C^r}^{k/r} \text{Lip}(f)^{\frac{k}{r}n} r_f(\epsilon/2, n, \mathscr{D}_\infty^k).$$

Hence, writing $\mathrm{lip}(f) := \max(\log \mathrm{Lip}(f), 0)$,

$$H^{k,C^r}_{\mathrm{top}}(f) \leq \frac{k}{r}\mathrm{lip}(f) + H^k_{\mathrm{top}}(f).$$

The inequality $H^{k,C^r}_{\mathrm{top}}(f) \geq H^k_{\mathrm{top}}(f)$ is obvious, concluding the proof.

Lemma 19. *The numbers $H^{k,C^r}_{\mathrm{top}}(f)$ do not depend on the underlying choice of a C^r size.*

Proof. Using Lemma 18, it is enough to treat the case with finite smoothness. Let $\mathscr{D}_1, \mathscr{D}_2$ be two standard families of k-disks, defined by two C^r sizes $\|\cdot\|^1_{C^r}, \|\cdot\|^2_{C^r}$. By Fact 56, there exists $C < \infty$ such that $\|\cdot\|^1_{C^r} \leq C\|\cdot\|^2_{C^r}$. Hence setting $K := ([C]+1)^k$, for any k-disk $\phi_1 \in \mathscr{D}_1$ can be *linearly subdivided*[2] into K k-disks $\phi_2^1, \ldots, \phi_2^K \in \mathscr{D}_2$. Thus

$$\forall n \geq 0 \quad r_f(\epsilon, n, \phi_1) \leq K \max_j r_f(\epsilon, n, \phi_2^j).$$

It follows immediately that $H(f, \mathscr{D}_1) \leq H(f, \mathscr{D}_2)$. The claimed equality follow in turn by symmetry.

4 Other Growth Rates of Submanifolds

4.1 Volume Growth

Entropy is a growth rate under iteration. Equipping M with a Riemannian structure allows the definition of volume growth of submanifolds.

Definition 20. Let $\phi : Q^k \to M$ be a singular k-disk. Its (*upper*) *growth rate* is:

$$\gamma(f, \phi) := \limsup_{n\to\infty} \frac{1}{n} \log \mathrm{vol}(f^n \circ \phi) \text{ with } \mathrm{vol}(\psi) := \int_{Q^k} \|\Lambda^k \psi(x)\|\, dx$$

where $\|\Lambda^k \psi\|$ is the Jacobian of $\psi : Q^k \to M$ wrt the obvious Riemannian structures. The volume growth exponent of f in dimension k is:

$$\gamma^k(f) := \sup_{\phi \in \mathscr{D}^k_r} \gamma(f, \phi),$$

$\gamma(f) := \max_{0\leq k\leq d} \gamma^k(f)$ is simply called the *volume growth* of f.

Observe that the value of the growth rates defined above are independent of the choice of the Riemannian structure, by compactness of the manifold.

The volume growth dominates the entropy quite generally:

[2] That is, each $\phi_2^j = \phi_1 \circ L_j$ with $L_j : Q^k \to Q^k$ linear and $\bigcup_{j=1}^K L_j(Q^k) = Q^k$.

Theorem 21 (Newhouse [23]). *Let $f : M \to M$ be a $C^{1+\alpha}$, $\alpha > 0$, smooth self-map of a compact manifold. Then:*

$$h_{\text{top}}(f) \leq \gamma(f).$$

Remark 22. More precisely, his proof gave

$$h_{\text{top}}(f) \leq \gamma^{d^{cu}}(f)$$

where d^{cu} is such that the variational principle $h_{\text{top}}(f) = \sup_\mu h(f, \mu)$ still holds when μ is restricted to measures with exactly d^{cu} nonpositive Lyapunov exponents.

For C^{1+1}-diffeomorphisms, deeper ergodic techniques due to Ledrappier and Young are available and Cogswell [11] has shown that, for any ergodic invariant probability measure μ, there exists a disk Δ such that $h_{\text{top}}(f, \mu) \leq h_{\text{top}}(f, \Delta) \leq \gamma(f, \Delta)$. More precisely, the dimension of this disk is the number of positive Lyapunov exponents. For C^∞ diffeomorphisms (more generally if there is a maximum measure) there exists a disk $\Delta_{\max}$ such that

$$h_{\text{top}}(f) = h_{\text{top}}(f, \Delta_{\max}) = \gamma(f, \Delta_{\max}).$$

I do not know if Newhouse's inequality fails for C^1 maps.

The proof of Newhouse inequality involves *ergodic theory* and especially *Pesin theory*. Indeed, this type of inequality does not hold uniformly:

Example 23. There exist a C^∞ self-map F of a surface and a C^∞ curve ϕ such that, for some sequence $n_i \to \infty$,

$$\lim_{i\to\infty} \frac{1}{n_i} \log r_F(\epsilon, n_i, \phi) > \lim_{i\to\infty} \frac{1}{n_i} \log \text{vol}(F^{n_i} \circ \phi).$$

Proof. Let $\alpha > 0$ be some small number. Let $I := [0, 1]$. Let $f : I \to I$ be a C^∞ map such that: (i) $f(0) = f(1) = 0$; (ii) $f(1/2) = 1$; (iii) $f|[0, 1/2]$ is increasing and $f|[1/2, 1]$ is decreasing; (iv) $f'|[0, 1/2 - \alpha] = 2(1 + \alpha)$ and $f'|[1/2 + \alpha] = -2(1+\alpha)$. As α is small, $1/2$ has a preimage in $[0, 1/2-\alpha]$. Let x_{-n} be the leftmost preimage in $f^{-n}(1)$: $x_0 = 1$, $x_{-1} = 1/2$, and for all $n \geq 2$, $x_{-n} = 2^{-n}(1+\alpha)^{-n+1}$. Let $g : I \to I$ be another C^∞ map such that: (i) $g(0) = 0$; (ii) $0 < g' < 1$; (iii) $g(x_{-n}) = x_{-n-1}$ for all $n \geq 0$.

Consider the following composition of length $3n$ for some $n \geq 1$:

$$I \longrightarrow^{f^n} 2^n \times I \longrightarrow^{g^n} 2^n \times [0, x_{-n}] \longrightarrow^{f^n} 2^n \times I. \tag{1}$$

Observe that after time $2n$, the length of the curve $g^n \circ f^n$ is $2^n \cdot x_{-n} = (1+\alpha)^{-n+1}$ whereas the number of (ϵ, n)-separated orbits is less than $\epsilon^{-1} n 2^n$. After time $3n$, the curve $f^n \circ g^n \circ f^n$ has image I with multiplicity 2^n. It is therefore easy to analyze the dynamics of compositions of such sequences.

We build our example by considering a skew-product for which the curve will be a fiber over a point which will drive the application of sequences as above.

Let $h : S^1 \to S^1$ be the circle map defined by $h(\theta) = 4\theta \bmod 2\pi$. Let $F : S^1 \times I \to S^1 \times I$ be a C^∞ map such that: $F(\theta, x) = (h(\theta), f(x))$ if $\theta \in [0, \frac{1}{6}]$ and $F(\theta, y) = (h(\theta), g(x))$ if $\theta \in [\frac{1}{2}, \frac{2}{3}]$.

Recall that the expansion in basis 4 of $\theta \in S^1$ is the sequence $a_1 a_2 \cdots \in \{0, 1, 2, 3\}^{\mathbb{N}}$ such that $\theta = 2\pi \sum_{k \geq 1} a_k 4^{-k}$. We write $\theta = \overline{0.a_1 a_2 a_3 \ldots}^4$.

Observe that, whenever θ has only 0s and 2s in its expansion,

$$h^n(\theta) \in \left[0, \frac{1}{6}\right] = [0, \overline{0.02222\ldots}^4]$$

whenever its nth digit is 0 and

$$h^n(\theta) \in \left[\frac{1}{2}, \frac{2}{3}\right] = [\overline{0.2000\ldots}^4, \overline{0.222\ldots}^4]$$

whenever its nth digit is 2. Thus we can specify the desired compositions of f and g just by picking $\theta \in S^1$ with the right expansion. We pick:

$$\theta_1 = \overline{0.0^{n_1} 2^{n_1} 0^{n_1+n_2} 2^{n_2} 0^{n_2+n_3} 2^{n_3} 0^{n_3+n_4} \ldots.}^4$$

so that we shall have a sequence of compositions of the type (1). We write $N_i := 3n_1 + \cdots + 3n_i$. We set $n_i := i!$ so that $n_{i+1}/N_i \to \infty$. Let $\phi^1 : Q^1 \to S^1 \times I$ be defined by $\phi^1(s) = (\theta_1, (s+1)/2)$.

The previous analysis shows that $F^{N_i} \circ \phi^1$ has image I with multiplicity $2^{n_1+\cdots+n_i} = 2^{\frac{1}{3}N_i}$. $F^{N_i+n_{i+1}} \circ \phi^1$ has image I with multiplicity $2^{\frac{1}{3}N_i} \times 2^{n_{i+1}}$. $F^{N_i+2n_{i+1}} \circ \phi^1$ has image $[0, x_{-n_{i+1}}]$ with multiplicity $2^{\frac{1}{3}N_i} \times 2^{n_{i+1}}$. It follows that, setting $t_i := N_i + 2n_{i+1} \approx 2n_{i+1}$,

$$\log r_F(\epsilon, t_i, \phi^1) \approx \left(\frac{1}{3}N_i + n_{i+1}\right) \log 2$$

whereas

$$\operatorname{vol}(F^{t_i} \circ \phi^1) = x_{-n_{i+1}} \times 2^{\frac{1}{3}N_i + n_{i+1}} = (1+\alpha)^{-n_{i+1}} 2^{\frac{1}{3}N_i}.$$

Hence,

$$\frac{1}{t_i} \log r_F(\epsilon, t_i, \phi^1) \approx \frac{1}{2} \log 2 \text{ whereas } \frac{1}{t_i} \log \operatorname{vol}(F^{t_i} \circ \phi^1) \preceq -\frac{1}{2}\alpha,$$

as claimed.

Remark 24. The inequality in the previous example is obtained as the length is contracted after a large expansion. For curves, this is in fact general and it is easily shown that, for any C^1 1-disk ϕ with unit length, for any $0 < \epsilon < 1$:

$$\forall n \geq 0 \quad \epsilon \cdot r_f(\epsilon, n, \phi) \leq \max_{0 \leq k < n} \operatorname{vol}(f^k \circ \phi) + 1. \tag{2}$$

Equation (2) implies that, for curves,

$$h_{\mathrm{top}}(f,\phi) \le \gamma(f,\phi), \tag{3}$$

both quantities being defined by lim sup (this would fail using lim inf). However, one can find similarly as above, a C^∞ self-map of a 3-dimensional compact manifold and a C^∞ smooth 2-disk such that (2) fails though (3) seems to hold.

We ask the following:

Question 25. Let $f : M \to M$ be a C^∞ self-map of a compact d-dimensional manifold. Is it true that, for any singular k-disk ψ ($0 \le k \le d$)

$$h_{\mathrm{top}}(f,\psi) \le \max_{\phi\subset\psi} \gamma(f,\phi)?$$

(both rates being defined using lim sup *and ϕ ranging over singular ℓ-disks, $0 \le \ell < k$, with $\phi(Q^\ell) \subset \psi(Q^k)$)? Is it at least true that*

$$h^k_{\mathrm{top}}(f) \le \max_{0\le\ell\le k} \gamma^\ell(f)?$$

These might even hold for finite smoothness for all I know.

Conversely, entropy also provides some bounds on volume growth

Theorem 26 (Yomdin [27]). *Let $f : M \to M$ be a C^r, $r \ge 1$, smooth self-map of a compact manifold. Let $\alpha > 0$. Then there exist $C(r,\alpha) < \infty$ and $\epsilon_0(r) > 0$ with the following property. Let $\phi : Q^k \to M$ be any C^r singular k-disk with unit C^r size for some $0 \le k \le d$. Then, for any $n \ge 0$,*

$$\mathrm{vol}(f^n \circ \phi) \le C(r,\alpha)\mathrm{Lip}(f)^{(\frac{k}{r}+\alpha)n} \cdot r_f(\epsilon_0, n, \phi).$$

In particular,

$$\gamma^k(f) \le h^k_{\mathrm{top}}(f) + \frac{k}{r}\mathrm{lip}(f).$$

Remark 27. The above extra term is indeed necessary as shown already by examples attributed by Yomdin [27] to Margulis: there is $f : [0,1] \to [0,1]$, C^r with $h_{\mathrm{top}}(f) = 0$ and $\gamma(f) = \mathrm{lip}(f)/r$.

Remark 28. Yomdin's estimate is *uniform* holding for each disk and each iterate. Its proof involves very little dynamics and no ergodic theory, in contrast to Newhouse's inequality quoted above.

Corollary 29. *Let $f : M \to M$ be a self-map of a compact manifold. If f is C^∞, then*

$$h_{\mathrm{top}}(f) = \gamma(f).$$

Let $f_* : H_*(M,\mathbb{R}) \to H_*(M,\mathbb{R})$ be the total homological action of f. Let $\rho(f_*)$ be its spectral radius. As the ℓ^1-norm in homology gives a lower bound on the volume, we have $\gamma(f) \ge \log \rho(f_*)$. Hence, the following special case of the Shub Entropy Conjecture is proved:

Corollary 30 (Yomdin [27]). *Let $f : M \to M$ be a self-map of a compact manifold. If f is C^∞, then*

$$\log \rho(f_*) \leq h_{\text{top}}(f).$$

4.2 Resolution Entropies

The previous results of Yomdin and more can be obtained by computing a growth rate taking into account the full structure of singular disks. A variant of this idea is explained in Gromov's Bourbaki Seminar [12] on Yomdin's results. We build on [4].

Definition 31. Let $r \geq 1$. Let $\phi : Q^k \to M$ be a C^r singular k-disk. A *C^r-resolution* $\mathscr{R}$ of order n of ϕ is a collection of C^r maps $\psi_\omega : Q^k \to Q^k$, for $\omega \in \Omega$ with Ω a finite collection of words of length $|\omega|$ at most n with the following properties. For each $\omega \in \Omega$, let $\Psi_\omega := \psi_{\sigma^{|\omega|-1}\omega} \circ \cdots \circ \psi_\omega(Q^k)$ (σ deletes the first symbol). We require:

1. $\bigcup_{|\omega|=n} \Psi_\omega(Q^k) = Q^k$;
2. $\|\psi_\omega\|_{C^r} \leq 1$ for all $\omega \in \Omega$;
3. $\|f^{|\omega|} \circ \Psi_\omega\|_{C^r} \leq 1$ for all $\omega \in \Omega$.

The *size* $|\mathscr{R}|$ of the resolution is the number of words in Ω with length n.

Condition (2) added in [4] much simplifies the link between resolutions and entropy. It no longer relies on Newhouse application of Pesin theory and becomes straightforward:

Fact 32 *Let $\mathscr{R} := \{\psi_\omega : Q^k \to Q^k : \omega \in \Omega\}$ be a C^r-resolution of order n of $\phi : Q^k \to M$. Let $\epsilon > 0$ and Q^k_ϵ be ϵ-dense in Q^k, i.e., $Q^k \subset \bigcup_{t \in Q^k_\epsilon} B(x, \epsilon)$. Then*

$$\{\Psi_\omega(t) : t \in Q^k_\epsilon \text{ and } \omega \in \Omega \text{ with } |\omega| = n\} \text{ is a } (\epsilon, n)\text{-cover of } \phi(Q^k).$$

On the other hand, the notion of resolution induces entropy-like quantities:

Definition 33. Let $1 \leq r < \infty$ and let $f : M \to M$ be a C^r self-map of a compact manifold. Let $R_f(C^r, n, \phi)$ be the minimal size of a C^r-resolution of order n of a C^r singular disk ϕ. The *resolution entropy* of ϕ is:

$$h_R(f, \phi) := \limsup_{n \to \infty} \frac{1}{n} \log R_f(C^r, n, \phi).$$

If $\mathscr{D}$ is a collection of C^r singular disks, its C^r resolution entropy is

$$h_{R,C^r}(f, \mathscr{D}) := \sup_{\phi \in \mathscr{D}} h_R(f, \phi)$$

and its C^r uniform resolution entropy is:

$$H_{R,C^r}(f, \mathscr{D}) := \limsup_{n \to \infty} \frac{1}{n} \log R_f(C^r, n, \mathscr{D})$$

where $R_f(C^r, n, \mathscr{D}) := \max_{\phi\in\mathscr{D}} R_f(C^r, n, \phi)$. We set:

$$h_R^{k,C^r}(f) = h_{R,C^r}(f, \mathscr{D}_r^k) \text{ and } H_R^{k,C^r}(f) = H_{R,C^r}(f, D_r^k).$$

The following is immediate but very important:

Fact 34 *Let $1 \le r < \infty$ and $0 \le k \le d$. Let $f : M \to M$ be a C^r self-map of a compact d-dimensional manifold. The sequence $n \mapsto R_f(C^r, n, D_r^k)$ is sub-multiplicative:*

$$R_f(C^r, n+m, D_r^k) \le R_f(C^r, n, D_r^k) R_f(C^r, m, D_r^k).$$

The key technical result of Yomdin's theory can be formulated as follows:

Proposition 35. *Let $1 \le r < \infty$ and $\alpha > 0$. Let $f : M \to M$ be a C^r self-map of a compact manifold. There exist constants C', $C(r,\alpha)$, $\epsilon_0(r,\alpha)$ with the following property. For any C^r singular disk ϕ, any number $0 < \epsilon < \epsilon_0(r,\alpha)$ and any integer $n \ge 1$,*

$$C'\epsilon^k r_f(\epsilon, n, \phi) \le R_f(C^r, n, \phi) \le C(r,\alpha)\mathrm{Lip}(f)^{(\frac{k}{r}+\alpha)n} r_f(\epsilon, n, \phi).$$

Remark that the above constants depend on f. The first inequality follows from Fact 32. The second is the core of Yomdin theory, we refer to [4] for details.

5 Properties of Dimensional Entropies

We turn to various properties of dimensional entropies, most of which can be shown using resolution entropy and its submultiplicativity.

5.1 Link between Topological and Resolution Entropies

We start by observing that Proposition 35 links the topological and resolution entropies.

Corollary 36. *For all positive integers r, k, any collection of C^r k-disks $\mathscr{D}$ and any C^r self-map f on a manifold equipped with a C^r size:*

$$h_{\mathrm{top}}(f, \mathscr{D}) \le h_{R,C^r}(f, \mathscr{D}) \le h_{\mathrm{top}}(f, \mathscr{D}) + \frac{k}{r}\log \mathrm{Lip}(f)$$
$$H_{\mathrm{top}}(f, \mathscr{D}) \le H_{R,C^r}(f, \mathscr{D}) \le H_{\mathrm{top}}(f, \mathscr{D}) + \frac{k}{r}\log \mathrm{Lip}(f).$$

If the disks in $\mathscr{D}$ are C^∞, then, for $r \le s < \infty$,

$$h_{R,C^r}(f,\mathscr{D}) \le h_{R,C^s}(f,\mathscr{D}) \le h_{\text{top}}(f,\mathscr{D}) + \frac{k}{s}\log \text{Lip}(f).$$

Letting $s \to \infty$, we get:

Corollary 37. *If f is C^∞, then, for all $1 \le r < \infty$,*

$$h_{R,C^r}(f,\mathscr{D}^k_\infty) = h_{\text{top}}(f,\mathscr{D}^k_\infty).$$

The same holds for uniform topological entropy.

5.2 Gap Between Uniform and Ordinary Dimensional Entropies

Yomdin theory gives the following relation:

Proposition 38. *Let $1 \le r < \infty$ and $f : M \to M$ be a C^r self-map of a compact d-dimensional manifold. For each $0 \le k \le d$,*

$$h^{k,C^r}_{\text{top}}(f) \le H^{k,C^r}_{\text{top}}(f) \le h^{k,C^r}_{\text{top}}(f) + \frac{k}{r}\text{lip}(f)$$

and the same holds for the resolution entropies $h^{k,C^r}_R(f)$ and $H^{k,C^r}_R(f)$.

In particular, in the C^∞ smooth case, all the versions of the dimensional entropies agree: $h^k_{\text{top}}(f) = H^k_{\text{top}}(f) = h^k_R(f) = H^k_R(f) = \lim_{r\to\infty} H^{k,C^r}_{\text{top}}(f)$.

Proof. It is obvious that the uniform entropies dominate ordinary ones. By Fact 32, $h^{k,C^r}_{\text{top}}(f) \le h^{k,C^r}_R(f)$ and $H^{k,C^r}_{\text{top}}(f) \le H^{k,C^r}_R(f)$. Therefore it is enough to show:

$$H^{k,C^r}_R(f) \le h^{k,C^r}_{\text{top}}(f) + \frac{k}{r}\text{lip}(f). \tag{4}$$

Let $\alpha > 0$. Let $\epsilon_0 > 0$ as in Proposition 35. This proposition defines a number $C(r,\alpha)$. By definition, for every $\phi \in D^k_r$, there exists $n_\phi < \infty$ such that

$$r_f(\epsilon_0, n_\phi, \phi) \le e^{(h^{k,C^r}_{\text{top}}(f)+\alpha)n_\phi}.$$

We can arrange it so that this holds for all k-disks ψ in some C^0 neighborhood $\mathscr{U}_\phi$ of ϕ. We also assume n_ϕ so large that $C(r,\alpha) \le e^{\alpha n_\phi}$.

By Proposition 35, each such ψ admits a resolution with size at most

$$r_f(\epsilon, n_\phi, \psi) \times C(r,\alpha)\text{Lip}(f)^{\frac{k}{r}n_\phi} \le e^{(h^{k,C^r}_R(f)+\frac{k}{r}\text{lip}(f)+2\alpha)n_\phi}.$$

D^k_r is relatively compact in the C^0 topology, hence there is a finite cover $D^k_r \subset \mathscr{U}_{\phi_1} \cup \cdots \cup \mathscr{U}_{\phi_K}$. Let $N := \max n_{\phi_j}$. It is now easy to build, for each $n \ge 0$ and each $\psi \in D^k_r$ a C^r resolution $\mathscr{R}$ of order n with:

$$|\mathscr{R}| \leq \exp\left(h_{\text{top}}^{k,C^r}(f) + \frac{k}{r}\text{lip}(f) + 2\alpha\right)(n+N).$$

Equation (4) follows by letting α go to zero.

5.3 Continuity Properties

Proposition 39. *We have the following upper semicontinuity properties*:

1. $f \mapsto H_R^{k,C^r}(f)$ *is upper semicontinuous in the* C^r *topology for all* $1 \leq r < \infty$;
2. $f \mapsto H_{\text{top}}^k(f)$ *is upper semicontinuous in the* C^∞ *topology*;
3. *the defect in upper semi-continuity of* $f \mapsto H_{\text{top}}^{k,C^r}(f)$ *at* $f = f_0$ *is at most* $\frac{k}{r}\text{lip}(f_0)$:

$$\limsup_{f \to f_0} H_{\text{top}}^{k,C^r}(f) \leq H_{\text{top}}^{k,C^r}(f_0) + \frac{k}{r}\text{lip}(f_0).$$

Proof. We prove (1). The sub-multiplicativity of resolution numbers observed in Fact 34 implies that: $H_R^{k,C^r}(f) = \inf_{n\geq 1} \frac{1}{n} \log R_f(C^r, n, D_r^k)$. For each fixed positive integer n, $R_g(C^r, n, D_r^k) \leq 2^k R_f(C^r, n, D_r^k)$ for any g C^r-close to f (use a linear subdivision). Thus $f \mapsto H_R^{k,C^r}(f)$ is upper semi-continuous in the C^r topology.

We deduce (3) from (1). Let $f_n \to f$ in the C^r topology. By the preceding, $H_R^{k,C^r}(f) \geq \limsup_{n\to\infty} H_R^{k,C^r}(f_n)$. By Proposition 38, $H_{\text{top}}^k(f) \geq H_R^{k,C^r}(f) - \frac{k}{r}\text{lip}(f)$.

(2) follows from (3) using Lemma 18.

On the other hand, $f \mapsto H_{\text{top}}^k(f)$ fails to be lower semi-continuous except for interval maps for which topological entropy is lower semi-continuous in the C^0 topology by a result of Misiurewicz. In every case there are counter examples:

Example 40. For any $d \geq 2$ and $1 \leq k \leq d$, there is a self-map of a compact manifold of dimension d at which $h_{\text{top}}^k(f)$ fails to be lower semi-continuous.

Let $h : \mathbb{R} \to [0,1]$ be a C^∞ function such that $h(t) = 1$ if and only if $t = 0$. Let $F_\lambda : [0,1]^d \to [0,1]^d$ be defined by

$$F_\lambda(x_1, \ldots, x_d) = (h(\lambda)x_1, 4x_1x_2(1-x_2), x_3, \ldots, x_d).$$

Observe that if $\lambda \neq 0$, then $h(\lambda) \in [0,1)$ and $F_\lambda^n(x_1, \ldots, x_d)$ approaches $\{(0,0)\} \times [0,1]^{d-2}$ on which F_λ is the identity. Therefore $h_{\text{top}}(F_\lambda) = 0$. On the other hand $h_{\text{top}}(F_0) = h_{\text{top}}(x \mapsto 4x(1-x)) = \log 2$. Now, $H_{\text{top}}^k(F_\lambda) \leq h_{\text{top}}(F_\lambda) = 0$ for any $\lambda \neq 0$ and $H_{\text{top}}^k(F_0) \geq h_{\text{top}}^k(f) \geq h_{\text{top}}(F_0, \{1\} \times [0,1] \times \{(0, \ldots, 0)\}) = \log 2$ for any $k \geq 1$.

6 Hyperbolicity from Entropies

We now explain how the dimensional entropies can yield dynamical consequences. We start by recalling an inequality which will yield hyperbolicity at the level of measures. Then we give the definition and main results for entropy-expanding maps. Finally we explain the new notion of entropy-hyperbolicity for diffeomorphisms.

6.1 A Ruelle-Newhouse Type Inequality

One of the key uses of dimensional entropies is to give bounds on the exponents using the following estimate. This will give hyperbolicity of large entropy measure from assumptions on these dimensional entropies.

Theorem 41 ([7]). *Let $f : M \to M$ be a C^r self-map of a compact manifold with $r > 1$. Let μ be an ergodic, invariant probability measure with Lyapunov exponents $\lambda_1(\mu) \geq \lambda_2(\mu) \geq \cdots \geq \lambda_d(\mu)$ repeated according to multiplicity. Recall that $H^k_{\text{top}}(f)$ is the uniform k-dimensional entropy of f. Then:*

$$h(f, \mu) \leq H^k_{\text{top}}(f) + \lambda_{k+1}(\mu)^+ + \cdots + \lambda_d(\mu)^+.$$

Remark 42. For $k = 0$ this reduces to Ruelle's inequality. For k equal to the number of nonnegative exponents, this is close to Newhouse inequality (with $H^k_{\text{top}}(f)$ replacing $\gamma^k(f)$). The proof is similar to Newhouse's and relies on Pesin theory.

6.2 Entropy-Expanding Maps

We require that the full topological entropy only appear at the full dimension.

Definition 43. A C^r self-map $f : M \to M$ of a compact manifold is *entropy-expanding* if:

$$H^{d-1}_{\text{top}}(f) < h_{\text{top}}(f).$$

An immediate class of examples is provided by the interval maps with non-zero topological entropy.

The first consequence of this condition is that ergodic invariant probability measures with entropy $> H^{d-1}_{\text{top}}(f)$ have only Lyapunov exponents bounded away from zero. This follows immediately from Theorem 41.

This also allows the application of (a non-invertible version of) Katok's theorem, proving a logarithmic lower bound on the number of periodic points.

Katok's proof gives horseshoes with topological entropy approaching $h_{\text{top}}(f)$. In particular these maps are points of lower semi-continuity of $f \mapsto h_{\text{top}}(f)$ in any C^r topology, $r \geq 0$. Combining with the upper semi-continuity from Yomdin theory we get:

Proposition 44. *The entropy-expansion property is open in the C^∞ topology.*

Thus we can use the following estimate

Proposition 45 ([6]). *The Cartesian product of a finite number of C^∞ smooth interval maps, each with nonzero topological entropy is entropy-expanding.*

To get dynamically interesting examples:

Example 46. For $|\epsilon|$ small enough, the plane map $F_\epsilon : (x, y) \mapsto (1 - 1.8x^2 - \epsilon y^2, 1 - 1.9y^2 - \epsilon x^2)$ preserves $[-1, 1]^2$ and its restriction to this set is entropy-expanding.

A sufficient condition, considered in a different approach by Oliveira and Viana [24, 25] is the following:

Lemma 47. *Let $f : M \to M$ be a diffeomorphism of a compact Riemanian manifold. Let $\|\Lambda^k Tf\|$ be the maximum over all $1 \leq \ell \leq k$ and all $x \in M$ of the Jacobian of the restrictions of the differential $T_x f$ to any k-dimensional subspace of $T_x M$. Then*

$$H^k_{\text{top}}(f) \leq \log \|\Lambda^k Tf\|.$$

In particular, $\log \|\Lambda^k T\| < h_{\text{top}}(f)$ implies that f is entropy-expanding. An even stronger condition is $(d-1)\text{lip}(f) < h_{\text{top}}(f)$.

The proof of this lemma is a variation on the classical proof of Ruelle's inequality.

We are able to analyze the dynamics of entropy-expanding maps with respect to large entropy measures rather completely.

Theorem 48. *Let $f : M \to M$ be a C^∞ self-map of a compact manifold. Assume that f is entropy-expanding. Then*:

- *f has finitely many maximum measures*;
- *Its periodic points satisfies a multiplicative lower bound.*

This can be understood as generalization of the Markov property which corresponds to partition having boundaries with essentially finite forward or backward orbits. The proof of the theorem involves a partition whose boundaries are pieces of smooth submanifolds, therefore of entropy bounded by $H^{d-1}_{\text{top}}(f)$.

In [9], we are able to define a nice class of symbolic systems, called *puzzles of quasi-finite type*, which contains the suitably defined symbolic representations of entropy-expanding maps satisfying a technical condition and have the above properties. Moreover, their periodic points define zeta functions with meromorphic extensions and their natural extensions can be classified up to entropy-conjugacy in the same way as interval maps.

6.3 Entropy-Hyperbolicity

Entropy-expanding maps are *never diffeomorphisms*. Indeed, they have ergodic invariant measures which have nonzero entropy and only positive Lyapunov exponents. Wrt the inverse diffeomorphism these measures have the same nonzero entropy but only negative Lyapunov exponents, contradicting Ruelle's inequality. Thus we need a different notion for diffeomorphism.

Definition 49. The *unstable* (*entropy*) *dimension* is:

$$d_u(f) := \min\{0 \le k \le d : H^k_{\text{top}}(f) = h_{\text{top}}(f)\}.$$

If f is a diffeomorphism, then the *stable dimension* is: $d_s(f) := d_u(f^{-1})$ (if f not a diffeomorphism we set $d_s(f) = 0$).

Observe that f is entropy-expanding if and only if $d_u(f)$ coincides with the dimension of the manifold.

Lemma 50. *Let $f : M \to M$ be a C^r self-map of a compact d-dimensional manifold with $r > 1$. Then:*

$$d_u(f) + d_s(f) \le d.$$

Proof. Theorem 41 implies that measures with entropy $> H^{d_u(f)-1}_{\text{top}}(f)$ have at least $d_u(f)$ positive exponents. The same reasoning applied to f^{-1} shows that such measures have at least $d_s(f)$ negative exponents. By the variational principle such measures exist. Hence $d_u(f) + d_s(f) \le d$.

We can now propose our definition:

Definition 51. A diffeomorphism such that $d_u(f) + d_s(f) = d$ is *entropy-hyperbolic*.

Obviously surface diffeomorphisms with non-zero topological entropy are entropy-hyperbolic.

Exactly as above, we obtain from Theorems 41 and 10:

Theorem 52. *Let $f : M \to M$ be a C^r diffeomorphism of some compact manifold with $r > 1$. Assume that f is entropy-hyperbolic. Then*:

- *All ergodic invariant probability measures with entropy close enough to the topological entropy have the absolute value of their Lyapunov exponents bounded away from zero*;
- *Their periodic points satisfy a logarithmic lower bound*;
- *They contain horseshoes with topological entropy arbitrarily close to that of f.*

Corollary 53. *The set of entropy-hyperbolic diffeomorphisms of a compact manifold is open in the C^∞ topology.*

6.4 Examples of Entropy-Hyperbolic Diffeomorphisms

The techniques of [6] yield:

Lemma 54. *Linear toral automorphisms are entropy-hyperbolic if and only if they are hyperbolic in the usual sense*: *no eigenvalue lies on the unit circle.*

The following condition is easily seen to imply entropy-hyperbolicity:

Lemma 55. *Let $f : M \to M$ be a diffeomorphism of a compact manifold of dimension d. Assume that there are two integers $d_1 + d_2 = d$ such that*:

$$\log \|\Lambda^{d_1-1} Tf\| < h_{\text{top}}(f) \text{ and } \log \|\Lambda^{d_2-1} Tf\| < h_{\text{top}}(f).$$

Then f is entropy-hyperbolic.

7 Further Directions and Questions

We discuss some developing directions and ask some questions.

7.1 Variational Principles

It seems reasonable to conjecture the following *topological variational principle* for dimensional entropies, at least for C^∞ self-maps and diffeomorphisms:

In each dimension, there is a C^∞ disk with maximum topological entropy, i.e., $h^k_{\text{top}}(f)$.

Does it fail for finite smoothness?

A probably more interesting but more delicate direction would be an *ergodic variational principle*. Even its formulation is not completely clear. A possibility would be as follows:

For each dimension k, $h^k_{\text{top}}(f)$ is the supremum of the entropies of k-disks contained in unstable manifolds of points in any set of full measure with respect to all invariant probability measures.

7.2 Dimensional Entropies of Examples

Let $f_i : M_i \to M_i$ are smooth maps for $i = 1, \ldots, n$ and consider the following formula:

$$H^k_{\text{top}}(f_1 \times \cdots \times f_n) = \max_{\ell_1+\cdots+\ell_n=k} H^{\ell_1}_{\text{top}}(f) + \cdots + H^{\ell_n}_{\text{top}}(f).$$

This is only known in special cases—see [3]. It would imply that product of entropy-expanding maps are again entropy-expanding.

If $f : M \to M$ is an expanding map of a compact manifold, is it true that $H_{\text{top}}^{d-1}(f) < h_{\text{top}}(f)$? Note that this fails for piecewise expanding maps (think of a limit set containing an isolated invariant curve with maximum entropy).

Likewise is an Anosov diffeomorphism, even far from linear, entropy-hyperbolic?

Find examples where $h_{\text{top}}^{k,C^r}(f) < H_{\text{top}}^{k,C^r}(f)$.

7.3 Other Types of Dimensional Complexity

Other "dimensional complexities" have been investigated from growth rates of multi(co)vectors for the Kozlovski entropy formula [21] to the currents which are fundamental to multidimensional complex dynamics [13] and the references therein.

How do they relate to the above dimensional entropies?

7.4 Necessity of Topological Assumptions

We have seen in Sect. 2.1 that, for maps, the assumption of no zero Lyapunov exponent for the large entropy measure, (or even that these exponents are bounded away from zero) is not enough for our purposes (e.g., finiteness of the number of maximum measures). Such results seem to require more uniform assumptions, like the one we make on dimensional entropies.

Is it the same for diffeomorphisms? That is, can one find diffeomorphisms with infinitely many maximum measures, all with exponents bounded away from zero?

Let f be a C^r self-map of a compact manifold. Assume that there are numbers $h < h_{\text{top}}(f)$, $\lambda > 0$, such that the Lyapunov exponents of any ergodic invariant measure with entropy at least h fall outside of $[-\lambda, \lambda]$. Assume also that the set of invariant probability measures with entropy $\geq h$ is compact. Does it follow that there are only finitely many maximum measures?

7.5 Entropy-Hyperbolicity

In a work in progress with T. Fisher, we show that the condition of Lemma 55 is satisfied by a version of a well-known example of robustly transitive, non-uniformly hyperbolic diffeomorphism of $\mathbb{T}^4$ due to Bonatti and Viana [1]. Building nice center-stable and center-unstable invariant laminations, we expect be able to show the same properties as in Theorem 48.

I however conjecture that the finite number of maximum measures, etc. should in fact hold for every C^∞ entropy-expanding diffeomorphism, even when there is no

such nice laminations. Of course this contains the case of surface diffeomorphisms which is still open (see Conjecture 9), despite the result on a toy model [8].

7.6 Generalized Entropy-Hyperbolicity

It would be interesting to have a *more general notion of entropy-hyperbolicity*. For instance, if a hyperbolic toral automorphism is entropy-hyperbolic, this is not the case for the disjoint union of two such systems of the same dimension if they have distinct stable dimensions. It may be possible to "localize" the definition either near points or near invariant measures to avoid these stupid obstructions (this is one motivation for the above question on variational principles for dimensional entropies).

If one could remove such obstructions, the remaining ones could reflect basic dynamical phenomena opening the door to a speculative "entropic Palis program".

8 C^r Sizes

We explain how to measure the C^r size of singular disks of a compact manifold M of dimension d. Here $1 \leq r \leq \infty$.

We select a finite atlas $\mathscr{A}$ made of charts $\chi_i : U_i \subset \mathbb{R}^d \to M$ such that changes of coordinates $\chi_i^{-1} \circ \chi_j$ are C^r-diffeomorphisms of open subsets of $\mathbb{R}^d$. Then we define, for any singular k-disk ϕ:

$$\|\phi\|_{C^r} := \sup_{x \in M} \inf_{U_i \ni x} \max_{s_1+\cdots+s_k \leq r} \max_{1 \leq j \leq d} |\partial_{t_1}^{s_1} \dots \partial_{t_k}^{s_k} (\pi_j \circ \chi_i \circ \phi)(t_1, \dots, t_k)|$$

where the above partial derivatives are computed at $t = \chi_i^{-1}(x)$ and $\pi_j(u_1, \dots, u_d) = u_j$.

Fact 56 *If $\|\cdot\|_{C^r}$ and $\|\cdot\|'_{C^r}$ are two C^r size defined by the above procedure, there exists a constant K such that, for any C^r k-disk $\phi : Q^k \to M$:*

$$\|\phi\|_{C^r} \leq K \cdot \|\phi\|'_{C^r}.$$

Fact 57 *Let $\phi : Q^k \to M$ be a C^r disk for some finite $r \geq 1$. Then, for any $t_0 \in Q^k$, there exists a C^∞ approximation $\phi_\infty : Q^k \to M$ such that*:

$$\forall t \in Q^k \quad d(\phi_\infty(t), \phi(t)) \leq \|\phi\|_{C^r} \|t - t_0\|^r,$$

and $\|\phi_\infty\|_{C^\infty} \leq 2\|\phi\|_{C^r}$.

This is easily shown by considering a neighborhood of $\phi(t_0)$ contained in a single chart of $\mathscr{A}$ and approximating ϕ by its Taylor expansion in that chart.

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The Scaling Limit of (Near-)Critical 2D Percolation

Federico Camia*

Abstract The geometric analysis of the continuum scaling limit of two-dimensional critical percolation has made tremendous progress in recent years. In this extended abstract, we give a brief introduction to scaling limits and summarize some of the recent progress in percolation. We discuss in particular how to obtain the scaling limit of the collection of all macroscopic cluster boundaries, and how one can attempt to use it to understand and study the scaling limit of percolation "near" the critical point.

1 Introduction

1.1 Critical Scaling Limits and SLE

One of the main goals of both probability theory and statistical physics is to understand and describe the large scale behavior of random systems consisting of many "microscopic" variables, where each single variable has a negligible effect and the behavior of the system is determined by the "sum" of all the variables. One usually wishes to study the behavior of such systems via some *observables*, suitably defined quantities that can be of an analytic or geometric nature. The asymptotic behavior of these quantities is often deterministic, but in some interesting cases it turns out to be random. Physicists and chemists have observed this type of macroscopic randomness in *critical systems*, i.e., systems at their phase transition point.

Federico Camia
Department of Mathematics, Vrije Universiteit Amsterdam, De Boelelaan 1081a, 1081 HV Amsterdam, The Netherlands, e-mail: fede@few.vu.nl

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In the theory of critical phenomena it is usually assumed that a physical system near a continuous phase transition is characterized by a single length scale (the *correlation length*) in terms of which all other lengths should be measured. When combined with the experimental observation that the correlation length diverges at the phase transition, this simple but strong assumption, known as the scaling hypothesis, leads to the belief that at criticality the system has no characteristic length, and is therefore invariant under scale transformations. This implies that all thermodynamic functions at criticality are homogeneous functions, and predicts the appearance of power laws.

It also suggests that for models of critical systems realized on a lattice, one can attempt to take a *continuum scaling limit* in which the mesh of the lattice is sent to zero while focus is kept on "macroscopic" observables that capture the large scale behavior. In the limit, the discrete model should converge to a continuum one that encodes the large scale properties of the original model, containing at the same time more symmetry. In many cases, this allows to derive extra insight by combining methods of discrete mathematics with considerations inspired by the continuum limit picture. The simplest example of such a continuum random model is Brownian motion, which is the scaling limit of the simple random walk. In general, though, the complexity of the discrete model makes it impossible even to guess the nature of the scaling limit, unless some additional feature can be shown to hold, which can be used to pin down properties of the continuum limit. Two-dimensional critical systems belong to the class of models for which this can be done, and the additional feature is *conformal invariance*.

In the eighties, physicists started exploring the consequences of conformal invariance. The constraints it poses on the continuum limits are particularly stringent in two dimensions, where every analytic function defines a conformal transformation (at points where its derivative is non-vanishing). A large number of critical problems in two dimensions were analyzed using conformal methods, including the Ising and Potts models, Brownian motion, the Self-Avoiding Walk (SAW), percolation, and Diffusion Limited Aggregation (DLA). The large body of knowledge and techniques that resulted, starting with the work of Belavin, Polyakov and Zamolodchikov [6, 7] in the early eighties, goes under the name of Conformal Field Theory (CFT). One of the main goals of CFT, and its most important application to statistical mechanics, is a complete classification of 2D critical systems in *universality classes* according to their scaling limit.

At the hands of theoretical physicists, CFT has been very successful in producing many interesting results. However, conformal invariance remains a conjecture for most models describing critical systems. Moreover, despite its success, CFT leaves a number of open problems. First of all, the theory deals primarily with *correlation functions* and quantities that are not directly expressible in terms of those are not easily accessible. Secondly, given some critical lattice model, there is no way, within the theory itself, of deciding to which CFT it corresponds. A third limitation, of a different nature, is due to the fact that the methods of CFT, although very powerful, are generally speaking not completely rigorous from a mathematical point of view.

Partly because of the success of CFT, in recent years work on critical phenomena had slowed down somewhat, probably due to the feeling that most of the leading problems had been resolved. In a somewhat surprising twist, the most recent developments in the area of two-dimensional critical systems have emerged in the mathematics literature, and have followed a completely new direction, which has provided new tools and a way of surpassing at least some of the limitations of CFT.

These developments came on the heels of interesting results on the scaling limits of discrete models (see, e.g., the work of Aizenman [1, 2], Benjamini-Schramm [8], Aizenman-Burchard [3], Aizenman-Burchard-Newman-Wilson [4], Aizenman-Duplantier-Aharony [5] and Kenyon [18, 19]) but they differ greatly from those because they are based on a radically new approach whose main tool is the Stochastic Loewner Evolution (SLE), or Schramm-Loewner Evolution, as it is also known, introduced by Schramm [28]. The new approach, which is probabilistic in nature, focuses directly on non-local structures that characterize a given system, such as cluster boundaries in Ising, Potts and percolation models, or loops in the $O(n)$ model. At criticality, these non-local objects become, in the continuum limit, random curves whose distributions can be uniquely identified thanks to their conformal invariance and a certain "Markovian" property. There is a one-parameter family of SLEs, indexed by a positive real number κ, and they appear to be essentially the only possible candidates for the scaling limits of interfaces of two-dimensional critical systems that are believed to be conformally invariant.

The identification of the scaling limit of interfaces of critical lattice models with SLE curves has led to tremendous progress in recent years. The main power of SLE stems from the fact that it allows to compute different quantities; for example, percolation crossing probabilities and various percolation critical exponents. Therefore, relating the scaling limit of a critical lattice model to SLE allows for a rigorous determination of some aspects of the large scale behavior of the lattice model. For the mathematician, the biggest advantage of SLE over CFT lies maybe in its mathematical rigor. But many physicists working on critical phenomena and CFT have promptly recognized the importance of SLE and added it to their toolbox.

In the context of the Ising, Potts and $O(n)$ models, as well as percolation, an SLE curve is believed to describe the scaling limit of a single interface, which can be obtained by imposing special boundary conditions. A single SLE curve is therefore not in itself sufficient to immediately describe the scaling limit of the unconstrained model without boundary conditions in the whole plane (or in domains with boundary conditions that do not determine a single interface), and contains only limited information concerning the connectivity properties of the model.

A more complete description can be obtained in terms of loops, corresponding to the scaling limit of cluster boundaries. Such loops should also be random and have a conformally invariant distribution, closely related to SLE. This observation led Wendelin Werner [35, 36] and Scott Sheffiled [29] to the definition of Conformal Loop Ensembles (CLEs), which are, roughly speaking, random collections of conformally invariant fractal loops. As for SLE, there is a one parameter family of CLEs.

The study of SLE and its connections to statistical mechanics is currently among the most active and rapidly growing areas of probability theory, and, especially in the work of Lawler, Scrhamm and Werner [20–24, 26, 25] has already provided many impressive (rigorous) results concerning various two-dimensional models such as Brownian motion, the *loop erased random walk* and the *uniform spanning tree*.

At present, there are at least three distinct directions into which research is developing. The first concerns the study of SLE itself (see [27]), a task that is being carried out by a growing number of mathematicians. Physicists on their part have used SLE to obtain information about CFT, and have also been active in reproducing certain SLE results with "traditional" CFT methods, thus pushing the boundaries of CFT. The hope in both the mathematics and physics community is that the interaction between SLE and CFT will continue to shed new light on both approaches and provide a deeper understanding of critical phenomena.

The third direction, which has been explored most notably by Lawler, Schramm and Werner [24, 26], Smirnov [30, 33, 31, 32], Smirnov and Werner [34], and Camia and Newman [12–15], consists in proving conformal invariance of the scaling limit for individual models of statistical mechanics, proving the convergence of interfaces in those models to SLE and CLE curves, and deriving information about the discrete models from their scaling limits.

The case of percolation is particularly illuminating because the connection with both SLE and CLE has been fully established and successfully exploited to derive rigorously several important results previously obtain by physicists using CFT methods. Moreover, the description of the "full" scaling limit, i.e., the scaling limit of *all* cluster boundaries, represents an important first step in understanding the near-critical scaling limit, when the system is slightly off-critical and it approaches criticality at an appropriate speed in the scaling limit.

1.2 Percolation

Percolation as a mathematical theory was introduced by Broadbent and Hammersley [10, 11] to model the spread of a gas or a fluid through a porous medium. To mimic the randomness of the medium, they declared the edges of the d-dimensional cubic lattice independently *open* (to the passage of the gas or fluid) with probability p or *closed* with probability $1 - p$. Since then, many variants of this simple model have been studied, attracting the interest of both mathematicians and physicists.

Mathematicians are interested in percolation because of its deceiving simplicity which hides difficult and elegant results. From the point of view of physicists, percolation is maybe the simplest statistical mechanical model undergoing a continuous phase transition as the value of the parameter p is varied, with all the standard features typical of critical phenomena (scaling laws, a conformally invariant scaling limit, universality). On the applied side, percolation has been used to model the spread of a disease, a fire or a rumor, the displacement of oil by water, the behav-

ior of random electrical circuits, and more recently the connectivity properties of communication networks.

In one version of the model, the vertices of the triangular lattice, identified with the hexagonal faces of its dual, the honeycomb lattice, are colored independently white with probability p or black otherwise. The questions regarding the geometry of this random coloring (for instance, whether there exists a path on white sites connecting the opposite edges of a large rectangle) can be expressed in terms of the behavior of clusters (i.e., maximal connected monochromatic subsets of the lattice) or of the boundaries between them.

It is well known that in this model if $p > 1/2$ (respectively, $p < 1/2$) there is an infinite white (respectively, black) cluster, while for $p = 1/2$ there is no infinite cluster of either color. The latter is the critical value of the model, at which the percolation phase transition occurs. Concerning the *critical behavior* of two-dimensional percolation, despite some important achievements, a complete and rigorous understanding had seemed out of reach until the introduction of SLE by Schramm [28] and the proof of conformal invariance of the scaling limit by Smirnov [30, 33].

2 The Critical Loop Process

2.1 General Features

At the percolation critical point, with probability one there is no infinite cluster (rigorously proved only in two and sufficiently high dimensions); therefore the percolation cluster boundaries form loops (see Fig. 1). We will refer to the continuum scaling limit (as the lattice spacing δ goes to zero) of the collection of all these loops as the *continuum nonsimple loop process*; its existence and some of its properties have been obtained in [12, 13]. We note that the cluster boundaries are naturally directed so that, for example, following a boundary according to its direction, white is to the left and black to the right. This gives to the collection of all boundaries a nested structure in which loops of opposite orientation alternate. The limiting (as $\delta \to 0$) loops also have this property.

The continuum nonsimple loop process can be described as a "conformally invariant gas" of loops, or more precisely, a conformally invariant probability measure on countable collections of continuous, nonsimple, noncrossing, fractal loops in the plane. It has the following properties, which are valid with probability one.

1. It is a random collection of countably many, noncrossing, continuous loops in the plane. The loops can and do touch themselves and each other many times, but there are no triple points; i.e. no three or more loops can come together at the same point, and a single loop cannot touch the same point more than twice, nor can a loop touch a point where another loop touches itself.
2. Any deterministic point z in the plane (i.e., chosen independently of the loop process) is surrounded by an infinite family of nested loops with diameters going

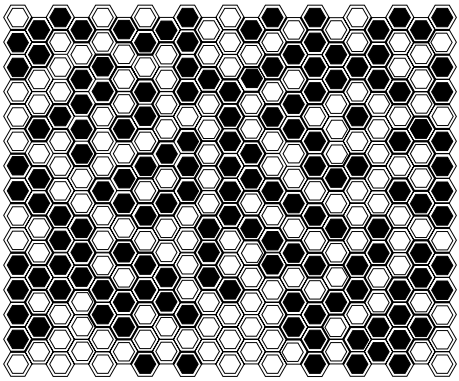

Fig. 1 Finite portion of a (site) percolation configuration on the triangular lattice with each hexagon representing a site. In the critical percolation model, the hexagons are colored black or white with equal probability. The cluster boundaries are indicated by heavy lines; some small loops appear, while other boundaries extend beyond the finite region depicted

to both zero and infinity; any annulus about that point with inner radius $r_1 > 0$ and outer radius $r_2 < \infty$ contains only a finite number $N(z, r_1, r_2)$ of those loops. Consequently, any two distinct deterministic points of the plane are separated by loops winding around each of them.

3. Any two loops are connected by a finite "path" of touching loops.

A continuum nonsimple loop process with the same distribution as the full scaling limit of critical percolation can be constructed directly by an inductive procedure in which each loop is obtained as the concatenation of an SLE_6 path with (a portion of) another SLE_6 path (see Sect. 2.2 below). In [12, 13] this procedure is carried out first inside a disc of radius R, and then the limit $R \to \infty$ is taken in order to obtain a measure on loops in the whole plane.

In [15], the scaling limit of the collection of all cluster boundaries contained in a generic Jordan domain D is considered, and it is shown that it gives rise to a Conformal Loop Ensemble (CLE) inside D.

2.2 Construction of a Single Loop

We will not give here the inductive construction of the full scaling limit, but in order to present some of the ideas of [12, 13] we explain how to construct a single loop by using two SLE_6 paths inside a domain D whose boundary is assumed to have a given orientation – see Fig. 2, where the orientation is clockwise. This is done in three steps, of which the first consists in choosing two points a and b on the boundary ∂D of D and "running" a chordal SLE_6, $\gamma(t) = \gamma_{D,a,b}(t)$, $t \in [0, 1]$, from a to b inside D. We consider $\gamma([0, 1])$ as an oriented path, with orientation from a to b. The set $D \setminus \gamma_{D,a,b}([0, 1])$ is a countable union of its connected components,

which are each open and simply connected. If z is a deterministic point in D, then with probability one, z is not touched by $\gamma([0, 1])$ [27] and so it belongs to a unique domain in $D \setminus \gamma([0, 1])$.

The components of $D \setminus \gamma([0, 1])$ can be conveniently thought of in terms of how a point z in the interior of the component was first "trapped" at some time t_1 by $\gamma([0, t_1])$, perhaps together with either $\partial_{a,b}D$ or $\partial_{b,a}D$ (the portions of the boundary ∂D from a to b counterclockwise or clockwise respectively): (1) those components whose boundary contains a segment of $\partial_{b,a}D$ between two successive visits at $\gamma_0(z) = \gamma(t_0)$ and $\gamma_1(z) = \gamma(t_1)$ to $\partial_{b,a}D$ (where here and below $t_0 < t_1$), (2) the analogous components with $\partial_{b,a}D$ replaced by the other part of the boundary, $\partial_{a,b}D$, (3) those components formed when $\gamma_0(z) = \gamma(t_0) = \gamma(t_1) = \gamma_1(z) \in D$ with γ winding about z in a counterclockwise direction between t_0 and t_1, and finally (4) the analogous clockwise components.

Now, let D' be a domain of type 1 (if ∂D were counterclockwise, we would take a domain of type 2) and let A and B be respectively the starting and ending point of the excursion $\mathcal{E}$ that generated D'. The second step to construct a loop is to run a chordal SLE_6, $\gamma' = \gamma_{D',B,A}$, inside D' from B to A; the third and final step consists in pasting together $\mathcal{E}$ and γ', keeping their orientations.

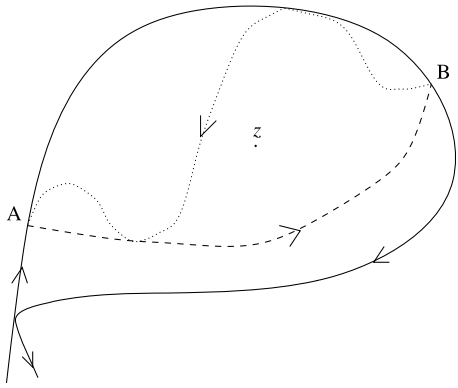

Fig. 2 Construction of a continuum loop around z in three steps. A domain D is formed by the solid curve. The dashed curve is an excursion $\mathcal{E}$ (from A to B) of an SLE_6 γ in D that creates a subdomain D' containing z. (Neither the rest of γ nor its starting and ending points, a and b, are indicated in the figure.) The dotted curve γ' is an SLE_6 in D' from B to A. A loop is formed by $\mathcal{E}$ followed by γ'

Running γ' inside D' from B to A partitions $D' \setminus \gamma'$ into new domains, all of whose boundaries have a well defined orientation, so that the construction of loops just presented can be iterated inside each one of these domains (as well as inside each of the domains of type 2, 3 and 4 generated by $\gamma_{D,a,b}$ in the first step). For the complete inductive procedure generating all the loops inside D, we refer the reader to [12, 13].

3 The Near-Critical Scaling Limit

Using the full scaling limit, one can attempt to understand the geometry of the near-critical scaling limit, where the percolation density tends to the critical one in an appropriate way as the lattice spacing δ tends to zero:

$$p = p_c + \lambda \delta^{\alpha} \tag{1}$$

where p_c is the critical density, δ is the lattice spacing, $\lambda \in (-\infty, \infty)$, and α is set equal to $1/\nu = 3/4$ (where ν is the correlation length exponent) to get nontrivial λ-dependence in the limit $\delta \to 0$ (as prescribed by "scaling theory," see also [1–3, 9]).

A heuristic analysis [16, 17] of the near-critical scaling limit leads to a one-parameter family of loop models (i.e., probability measures on random collections of loops), with the critical full scaling limit corresponding to a particular choice of the parameter ($\lambda = 0$). Except for the latter case, these measures are not scale invariant, but are mapped into one another by scale transformations.

The approach proposed in [16, 17] is based on a "Poissonian marking" of double points of the critical full scaling limit of [12, 13], i.e., points where two loops touch each other or a loop touches itself. These double points of the loop process in the plane are precisely the continuum limit of "macroscopically pivotal" lattice locations; each such site is microscopic, but such that a change in its state (e.g., black to white or closed to open) has a macroscopic effect on connectivity. For site percolation on the triangular lattice (or equivalently random black/white colorings of the hexagonal lattice – see Fig. 1), a macroscopically pivotal site is a hexagon at the center of four macroscopic arms with alternating colors – see Fig. 3.

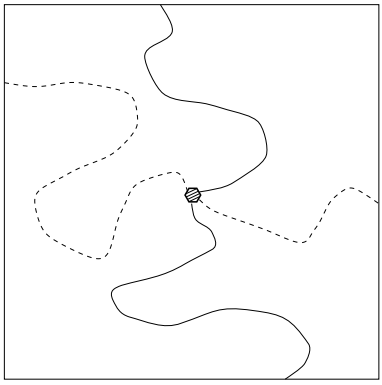

Fig. 3 Schematic diagram of a macroscopically pivotal hexagon at the center of four macroscopic arms with alternating color. The full and dashed lines represent paths of white and black hexagons respectively

The analysis presented in [16, 17] is based on the random marking of countably many double points, with each of these labelled by a number in $(-\infty, \infty)$ representing the value of λ at which that double point changes its state and hence correspondingly changes the macroscopic connectivity. This yields a realization on a single probability space of all the scaling limits as λ varies in $(-\infty, \infty)$. We point out that most double points are not marked since they do not change their state for a finite value of λ (in the limit $\delta \to 0$) – it is only the marked ones that change.

This approach can be used to define a renormalization group flow (under the action of dilations), and to describe the scaling limit of related models, such as invasion and dynamical percolation and the minimal spanning tree. In particular, this analysis helps explain why the scaling limit of the minimal spanning tree may be scale invariant but *not* conformally invariant, as first observed numerically by Wilson [37].

In [16, 17] some geometric properties of the near-critical scaling limit of two-dimensional percolation are conjectured, including the fact that for any $\lambda \neq 0$, every deterministic point of the plane is almost surely surrounded by a largest loop and by a countably infinite family of nested loops with radii going to zero (to be contrasted with the case of the *critical* full scaling limit, $\lambda = 0$, where there is no largest loop around any point).

The analysis done in [16, 17] is nonrigorous, and the purpose of the authors is not to prove theorems but rather to propose a *conceptual* framework rich enough to treat scaling limits of near-critical percolation and of related lattice objects like the minimal spanning tree.

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Black Hole Entropy Function and Duality

Gabriel Lopes Cardoso

Abstract The macroscopic entropy and the attractor equations for extremal black hole solutions follow from a variational principle based on an entropy function. We review this variational principle for static extremal black holes in four space-time dimensions and we apply it to $N = 2$ supergravity theories with higher-curvature interactions.

1 Introduction

String theory provides a microscopic derivation of the macroscopic Bekenstein-Hawking entropy of certain supersymmetric black holes [21]. An important feature of supersymmetric black holes is that they are charged and are supported by scalar fields. In the black hole background these scalar fields vary radially as one moves from spatial infinity to the horizon of the black hole, and they get attracted to specific values at the horizon which are determined by the black hole charges. This is the so-called attractor mechanism, which was first studied in [10, 20, 9, 8]. As a result, the macroscopic entropy is entirely determined in terms of the black hole charges and can be compared with the microscopic entropy based on state counting. The attractor mechanism is, however, not just a feature of supersymmetric black holes, but is also present for extremal non-supersymmetric black holes [11, 12, 18, 13]. The attractor behaviour is encoded in a set of attractor equations, which can be obtained by extremizing a so-called entropy function [18]. In addition, the value of this function at the extremum yields the macroscopic entropy of the extremal black hole.

We review the entropy function for static extremal black hole solutions in four space-time dimensions using the approach of [5] based on electric/magnetic duality

Gabriel Lopes Cardoso
Arnold Sommerfeld Center for Theoretical Physics, Department für Physik, Ludwig-Maximilians-Universität München, Munich, Germany, e-mail: gcardoso@theorie.physik.uni-muenchen.de

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covariance. Then, following [17], we specialize to the case of $N = 2$ supergravity theories with higher-curvature interactions. We also review the construction of a duality invariant OSV integral formula for supersymmetric black holes [4]. We refer to [5, 4] for a detailed discussion of these topics.

2 Entropy Function and Electric/Magnetic Duality Covariance

Let us consider static extremal black hole solutions to the equations of motion of a general system of Abelian vector gauge fields, scalar and matter fields coupled to gravity in four space-time dimensions. Following [18], we take the near-horizon geometry of such a black hole to be of the form $AdS_2 \times S^2$. Thus, we consider near-horizon solutions with spherical symmetry, which may be written as

$$\begin{aligned} \mathrm{d}s^2_{(4)} &= g_{\mu\nu}\mathrm{d}x^\mu \mathrm{d}x^\nu = v_1\Big(-r^2\,\mathrm{d}t^2 + \frac{\mathrm{d}r^2}{r^2}\Big) + v_2\big(\mathrm{d}\theta^2 + \sin^2\theta\,\mathrm{d}\varphi^2\big), \\ F^I_{rt} &= e^I, \qquad F^I_{\theta\varphi} = \frac{p^I}{4\pi}\sin\theta. \end{aligned} \tag{1}$$

Here the $F^I_{\mu\nu}$ denote the field strengths associated with a number of Abelian gauge fields. The θ-dependence of $F^I_{\theta\varphi}$ is fixed by rotational invariance and the p^I denote the magnetic charges. The fields e^I are dual to the electric charges. In addition to the constant fields e^I, v_1 and v_2 there may be a number of other fields which for the moment we denote collectively by u_α.

As is well known theories based on Abelian vector fields are subject to electric/magnetic duality, because their equations of motion expressed in terms of the dual field strengths,[1]

$$G_{\mu\nu I} = \sqrt{|g|}\varepsilon_{\mu\nu\rho\sigma}\frac{\partial\mathcal{L}}{\partial F^I_{\rho\sigma}}, \tag{2}$$

take the same form as the Bianchi identities for the field strengths $F^I_{\mu\nu}$. Adopting the conventions where $x^\mu = (t, r, \theta, \varphi)$ and $\varepsilon_{tr\theta\varphi} = 1$, and the signature of the space-time metric equals $(-,+,+,+)$, it follows that, in the background (1),

$$\begin{aligned} G_{\theta\varphi I} &= -v_1 v_2 \sin\theta\frac{\partial\mathcal{L}}{\partial F^I_{rt}} = -v_1 v_2\sin\theta\frac{\partial\mathcal{L}}{\partial e^I}, \\ G_{rtI} &= -v_1 v_2 \sin\theta\frac{\partial\mathcal{L}}{\partial F^I_{\theta\varphi}} = -4\pi\, v_1 v_2\frac{\partial\mathcal{L}}{\partial p^I}. \end{aligned} \tag{3}$$

[1] Here and henceforth we assume that the Lagrangian depends on the Abelian field strengths but not on their space-time derivatives. We also assume that the gauge fields appear exclusively through their field strengths.

These two tensors can be written as $q_I \sin\theta/(4\pi)$ and f_I. The quantities q_I and f_I are conjugate to p^I and e^I, respectively, and can be written as

$$\begin{aligned} q_I(e, p, v, u) &= -4\pi v_1 v_2 \frac{\partial \mathcal{L}}{\partial e^I}, \\ f_I(e, p, v, u) &= -4\pi v_1 v_2 \frac{\partial \mathcal{L}}{\partial p^I}. \end{aligned} \tag{4}$$

The q_I are constant by virtue of the equations of motion and correspond to the electric charges. Electric/magnetic duality transformations are induced by rotating the tensors $F^I_{\mu\nu}$ and $G_{\mu\nu\, I}$ by a constant transformation, so that the new linear combinations are all subject to Bianchi identities. This leads to new quantities $(\tilde{p}^I, \tilde{q}_I)$ and $(\tilde{e}^I, \tilde{f}_I)$.

Next, we define the reduced Lagrangian by the integral of the full Lagrangian over the horizon two-sphere S^2,

$$\mathcal{F}(e, p, v, u) = \int \mathrm{d}\theta\, \mathrm{d}\varphi \sqrt{|g|}\mathcal{L}. \tag{5}$$

We note that the definition of the conjugate quantities q_I and f_I takes the form,

$$q_I = -\frac{\partial \mathcal{F}}{\partial e^I}, \qquad f_I = -\frac{\partial \mathcal{F}}{\partial p^I}. \tag{6}$$

It is known that a Lagrangian does not transform as a function under electric/magnetic dualities. Instead we have [6],

$$\tilde{\mathcal{F}}(\tilde{e}, \tilde{p}, v, u) + \frac{1}{2}[\tilde{e}^I \tilde{q}_I + \tilde{f}_I \tilde{p}^I] = \mathcal{F}(e, p, v, u) + \frac{1}{2}[e^I q_I + f_I p^I] \tag{7}$$

so that the linear combination $\mathcal{F}(e, p, v, u) + \frac{1}{2}[e^I q_I + f_I p^I]$ transforms as a function. It is easy to see that the combination $e^I q_I - f_I p^I$ transforms as a function as well, so that we may construct a modification of (5) that no longer involves the f_I and that transforms as a function under electric/magnetic duality,

$$\mathcal{E}(q, p, v, u) = -\mathcal{F}(e, p, v, u) - e^I q_I, \tag{8}$$

which takes the form of a Legendre transform in view of the first equation (6). In this way we obtain a function of electric and magnetic charges. Therefore it transforms under electric/magnetic duality according to $\tilde{\mathcal{E}}(\tilde{q}, \tilde{p}, v, u) = \mathcal{E}(q, p, v, u)$. Furthermore the field equations imply that the q_I are constant and that the action, $\int \mathrm{d}t\mathrm{d}r\, \mathcal{E}$, is stationary under variations of the fields v and u, while keeping the p^I and q_I fixed. This is to be expected as $\mathcal{E}$ is in fact the analogue of the Hamiltonian density associated with the reduced Lagrangian density (5), at least as far as the vector fields are concerned. The constant values of the fields $v_{1,2}$ and u_α are thus determined by demanding $\mathcal{E}$ to be stationary under variations of v and u,

$$\frac{\partial \mathcal{E}}{\partial v} = \frac{\partial \mathcal{E}}{\partial u} = 0. \tag{9}$$

The function $2\pi\, \mathcal{E}(q,\, p,\, v,\, u)$ coincides with the entropy function proposed by Sen [18]. Equation (9) is the so-called attractor equation and the macroscopic entropy is directly proportional to the value of $\mathcal{E}$ at the stationary point,

$$\mathcal{S}_{\rm macro}(p,q) \propto \mathcal{E}\Big|_{\rm attractor}. \tag{10}$$

The above derivation of the entropy function applies to any gauge and general coordinate invariant Lagrangian, and, in particular, also to Lagrangians containing higher-derivative interactions. The entropy computed by (10) is Wald's entropy [22, 14, 15] which, in the absence of higher-derivative interactions, reduces to the area law of Bekenstein and Hawking.

In the absence of higher-derivative terms, the reduced Lagrangian $\mathcal{F}$ is at most quadratic in e^I and p^I and the Legendre transform (8) can easily be carried out. For instance, consider the following Lagrangian in four space-time dimensions (we only concentrate on terms quadratic in the field strengths),

$$\mathcal{L}_0 = -\frac{1}{4}\{\mathcal{N}_{IJ} F^{+I}_{\mu\nu} F^{+\mu\nu J} - \bar{\mathcal{N}}_{IJ} F^{-I}_{\mu\nu} F^{-\mu\nu J}\}, \tag{11}$$

where $F^{\pm I}_{\mu\nu}$ denote the (anti)-selfdual field strengths. In the context of this paper the tensors $F^{\pm I}_{\underline{rt}} = \pm \mathrm{i} F^{\pm I}_{\underline{\theta\varphi}} = \frac{1}{2}(F^I_{\underline{rt}} \pm \mathrm{i} F^I_{\underline{\theta\varphi}})$ are relevant, where underlined indices refer to the tangent space. It is straightforward to evaluate the entropy function (8) in this case,

$$\mathcal{E} = -\frac{v_1}{8\pi v_2}(q_I - \mathcal{N}_{IK} p^K)[(\mathrm{Im}\,\mathcal{N})^{-1}]^{IJ}(q_J - \bar{\mathcal{N}}_{JL} p^L), \tag{12}$$

which is indeed compatible with electric/magnetic duality. Upon decomposing into real matrices, $\mathrm{i}\mathcal{N}_{IJ} = \mu_{IJ} - \mathrm{i}\nu_{IJ}$, this result coincides with the corresponding terms in the so-called black hole potential

$$V_{\rm BH} = \frac{1}{2}(p,q)^T \mathcal{M} \begin{pmatrix} p \\ q \end{pmatrix}, \qquad \mathcal{M} = \begin{pmatrix} \mu + \nu\mu^{-1}\nu & \nu\mu^{-1} \\ \mu^{-1}\nu & \mu^{-1} \end{pmatrix}, \tag{13}$$

discussed in [11], and more recently in [13]. Namely, setting $v_1 = v_2$ (which enforces the vanishing of the curvature scalar) we obtain $\mathcal{E} = (4\pi)^{-1} V_{\rm BH}$.

3 Application to $N = 2$ Supergravity

We now give the entropy function for $N = 2$ supergravity coupled to n Abelian $N = 2$ vector multiplets, first at the two-derivative level and then in the presence of higher-curvature interactions proportional to the square of the Weyl tensor. Here we

follow the conventions of [3], where the charges and the Lagrangian have different normalizations than in the previous section.

The $N = 2$ vector multiplets contain complex physical scalar fields which we denote by X^I, $I = 0, \ldots, n$. At the two-derivative-level, the action for the vector multiplets is encoded in a holomorphic function $F(X)$. The coupling to supergravity requires this function to be homogeneous of second degree, i.e. $F(\lambda X) = \lambda^2 F(X)$. The gauge coupling functions $\mathcal{N}_{IJ}$ in (11) are given in terms of derivatives of $F(X)$,

$$\mathcal{N}_{IJ} = \bar{F}_{IJ} + 2\mathrm{i}\frac{\mathrm{Im}F_{IK}\mathrm{Im}F_{JL}X^K X^L}{\mathrm{Im}F_{MN}X^M X^N}, \tag{14}$$

where $F_I = \partial F(X)/\partial X^I$ and $F_{IJ} = \partial^2 F(X)/\partial X^I \partial X^J$.

Imposing the vanishing of the Ricci scalar, i.e. setting $v_1 = v_2$, the resulting entropy function (12) can be brought into the equivalent form [5],

$$\mathcal{E} = \frac{1}{2}\Sigma + \frac{1}{2}N^{IJ}(\mathcal{Q}_I - F_{IK}\mathcal{P}^K)(\mathcal{Q}_J - \bar{F}_{JL}\mathcal{P}^L), \tag{15}$$

where

$$\Sigma = -\mathrm{i}\left(\bar{Y}^I F_I - Y^I \bar{F}_I\right) - q_I(Y^I + \bar{Y}^I) + p^I(F_I + \bar{F}_I), \tag{16}$$

and

$$\begin{aligned} \mathcal{P}^I &\equiv p^I + \mathrm{i}(Y^I - \bar{Y}^I), \\ \mathcal{Q}_I &\equiv q_I + \mathrm{i}(F_I - \bar{F}_I). \end{aligned} \tag{17}$$

Here the Y^I are related to the X^I by a uniform rescaling and F_I denotes the derivative of $F(Y)$ with respect to Y^I. Also $N_{IJ} = \mathrm{i}(\bar{F}_{IJ} - F_{IJ})$, where $F_{IJ} = \partial^2 F(Y)/\partial Y^I \partial Y^J$.

Varying the entropy function (15) with respect to the scalar fields Y^I yields the attractor equations

$$\begin{aligned} &\left(\mathcal{Q}_I - F_{IJ}\mathcal{P}^J\right) - \frac{\mathrm{i}}{2}\left(\mathcal{Q}_K - \bar{F}_{KM}\mathcal{P}^M\right)N^{KP}F_{PIQ}N^{QL}\left(\mathcal{Q}_L - \bar{F}_{LN}\mathcal{P}^N\right) \\ &\quad = 0, \end{aligned} \tag{18}$$

where $F_{PIQ} = \partial^3 F(Y)/\partial Y^P \partial Y^I \partial Y^Q$. The attractor equations determine the horizon value of the Y^I in terms of the black hole charges (p^I, q_I). Because the function $F(Y)$ is homogeneous of second degree, we have $F_{IJK}Y^K = 0$. Using this relation one deduces from (18) that $(\mathcal{Q}_J - F_{JK}\mathcal{P}^K)Y^J = 0$, which is equivalent to

$$\mathrm{i}(\bar{Y}^I F_I - Y^I \bar{F}_I) = p^I F_I - q_I Y^I. \tag{19}$$

Therefore, at the attractor point, we have

$$\Sigma = \mathrm{i}(\bar{Y}^I F_I - Y^I \bar{F}_I). \tag{20}$$

It is possible to incorporate higher-curvature interactions involving the square of the Weyl tensor by including the Weyl multiplet into the function F, so that now $F = F(Y, \Upsilon)$ subject to

$$F(\lambda Y, \lambda^2 \Upsilon) = \lambda^2 F(Y, \Upsilon). \tag{21}$$

Here Υ denotes the rescaled square of the auxiliary field T_{ab} of the Weyl multiplet. The associated entropy function is then given by [5]

$$\begin{aligned}\mathcal{E}(Y, \bar{Y}, \Upsilon, U) = \frac{1}{2} U \Sigma + \frac{1}{2} U N^{IJ} (\mathcal{Q}_I - F_{IK} \mathcal{P}^K)(\mathcal{Q}_J - \bar{F}_{JL} \mathcal{P}^L) \\ - \frac{4\mathrm{i}}{\sqrt{-\Upsilon}} (\bar{Y}^I F_I - Y^I \bar{F}_I)(U - 1) \\ - \mathrm{i}(F_\Upsilon - \bar{F}_\Upsilon)\big[- 2U\Upsilon + 32(U + U^{-1} - 2) \\ - 8(1 + U)\sqrt{-\Upsilon}\big],\end{aligned} \tag{22}$$

where now

$$\Sigma = \mathcal{F}(Y, \bar{Y}, \Upsilon, \bar{\Upsilon}) - q_I (Y^I + \bar{Y}^I) + p^I (F_I + \bar{F}_I). \tag{23}$$

The quantity $\mathcal{F}(Y, \bar{Y}, \Upsilon, \bar{\Upsilon})$ is defined by

$$\mathcal{F}(Y, \bar{Y}, \Upsilon, \bar{\Upsilon}) = -\mathrm{i} \left(\bar{Y}^I F_I - Y^I \bar{F}_I \right) - 2\mathrm{i} \left(\Upsilon F_\Upsilon - \bar{\Upsilon} \bar{F}_\Upsilon \right), \tag{24}$$

where $F_\Upsilon = \partial F / \partial \Upsilon$. The entropy function (22) depends on the variables $U = v_1/v_2$, Υ and Y^I. Their attractor values are determined by requiring $\mathcal{E}$ to be stationary. We refer to [5] for the detailed form of the associated attractor equations.

With the normalizations used in this section, the entropy (10) reads

$$\mathcal{S}_{\text{macro}}(p, q) = 2\pi \mathcal{E} \Big|_{\text{attractor}}. \tag{25}$$

Supersymmetric black holes are the subset of extremal black holes satisfying [3]

$$\mathcal{Q}_I = \mathcal{P}^J = 0, \qquad \Upsilon = -64, \qquad U = 1. \tag{26}$$

The conditions $\mathcal{Q}_I = \mathcal{P}^J = 0$ can also be obtained from a variational principle based on Σ [1, 4]. The entropy of supersymmetric black holes reads [2]

$$\mathcal{S}_{\text{macro}} = \pi \Sigma|_{\text{attractor}}. \tag{27}$$

It can be written as a Legendre transform [16],

$$\mathcal{S}_{\text{macro}} = \pi \left[\mathcal{F}_E(p, \phi) - q_I \phi^I \right], \tag{28}$$

where

$$\mathcal{F}_E(p, \phi) = 4\mathrm{Im}\, F(Y, \Upsilon = -64), \tag{29}$$

with

$$Y^I = \frac{1}{2}\left(\phi^I + \mathrm{i}p^I\right) \tag{30}$$

and the ϕ^I satisfying the attractor equations $q_I = \partial \mathcal{F}_E/\partial \phi^I$.

4 Duality Invariant OSV Integral

The quantity Σ given above can be used to define a duality invariant version of the OSV integral for supersymmetric black holes. The OSV conjecture expresses microscopic state degeneracies $d(q, p)$ in terms of macroscopic data [16],

$$d(p,q) \propto \int \mathrm{d}\phi \mathrm{e}^{\pi[\mathcal{F}_{\mathrm{E}}(p,\phi) - q_I\phi^I]}, \tag{31}$$

where $\mathcal{F}_{\mathrm{E}}(p, \phi)$ was defined in (29). Electric/magnetic duality is, however, not manifest in (31). A duality invariant version of the OSV integral can be constructed using (23), with Υ set to its attractor value $\Upsilon = -64$. It reads [4]

$$d(p,q) \propto \int \mathrm{d}Y \mathrm{d}\bar{Y}\, \Delta(Y,\bar{Y}) \mathrm{e}^{\pi\Sigma(Y,\bar{Y},p,q)}, \tag{32}$$

where $\Delta = |\det \mathrm{Im} F_{KL}|$ (non-holomorphic corrections to the coupling functions can also be incorporated into (32)). Integrating (32) over fluctuations $\delta(Y^I - \bar{Y}^I)$ in saddle-point approximation results in [4]

$$d(p,q) \propto \int \mathrm{d}\phi \sqrt{\Delta(p,\phi)} \mathrm{e}^{\pi[\mathcal{F}_{\mathrm{E}}(p,\phi) - q_I\phi^I]}, \tag{33}$$

which is a modified version of the OSV integral (31), containing a non-trivial integration measure factor $\sqrt{\Delta}$ which is necessary for consistency with electric/magnetic duality. Evaluating (33) further in saddle-point approximation precisely yields the macroscopic entropy (27). The presence of the measure factor in (33) has been confirmed in the recent works [19, 7].

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Weak Turbulence for Periodic NLS

James Colliander

Abstract This paper summarizes a talk given in the PDE Session at the 2006 International Congress on Mathematical Physics about joint work with M. Keel, G. Staffilani, H. Takaoka and T. Tao. We build new smooth solutions of the cubic defocussing nonlinear Schrödinger equation on the two dimensional torus which are weakly turbulent: given any $\delta \ll 1$, $K \gg 1$, $s > 1$, we construct smooth initial data u_0 in the Sobolev space H^s with $\|u_0\|_{H^s} < \delta$, so that the corresponding time evolution u satisfies $\|u(T)\|_{H^s} > K$ at some time T.

1 Introduction

This note describes aspects of joint work with M. Keel, G. Staffilani, H. Takaoka and T. Tao appearing in [3]. We study the initial value problem for the cubic defocussing nonlinear Schrödinger (*NLS*) equation

$$\begin{cases} -i\partial_t u + \Delta u = |u|^2 u \\ u(0,x) = u_0(x) \end{cases} \tag{1}$$

where $u(t,x)$ is a $\mathbb{C}$-valued function with $x \in \mathbb{T}^2 = \mathbb{R}^2/(2\pi\mathbb{Z})^2$. Smooth solutions of (1) satisfy energy conservation,

$$E[u](t) = \int_{\mathbb{T}^2} \frac{1}{2}|\nabla u|^2 + \frac{1}{4}|u|^4 dx(t) = E[u_0] \tag{2}$$

and mass conservation,

James Colliander
Department of Mathematics, University of Toronto, Bahen Centre, Toronto, Ontario M5S 3G3, Canada, e-mail: colliand@math.toronto.edu

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$$\int_{\mathbb{T}^2} |u|^2 dx(t) = \int_{\mathbb{T}^2} |u_0|^2 dx, \tag{3}$$

for all $t > 0$. The local well-posedness result of Bourgain [1] for data $u_0 \in H^s(\mathbb{T}^2)$, $s > 0$, and these conservation laws imply the existence of a unique global smooth solution to (1) evolving from smooth initial data.

The main result of the paper is the construction of solutions to (1) with arbitrarily large growth in high Sobolev norms:

Theorem 1. *Let $1 < s$, $K \gg 1$, and $0 < \delta \ll 1$ be given parameters. Then there exists a global smooth solution $u(t, x)$ to (1) and a time $T > 0$ with*

$$\|u(0)\|_{H^s} \leq \delta$$

and

$$\|u(T)\|_{H^s} \geq K.$$

Using the conservation laws, we have an H^1-stability property near zero,

$$\left(\limsup_{|t|\to\infty} \left[\sup_{\|u_0\|_{H^1} \leq \delta} \|u(t)\|_{H^1} \right] \right) \leq C\delta.$$

Theorem 1 implies a different behavior in the range $s > 1$. Since δ may be chosen to be arbitrarily small and K may be chosen arbitrarily large, we observe that (1) is strongly unstable in H^s near zero for all $s > 1$:

$$\inf_{\delta>0} \left(\limsup_{|t|\to\infty} \left[\sup_{\|u_0\|_{H^s} \leq \delta} \|u(t)\|_{H^s} \right] \right) = \infty. \tag{4}$$

It remains an open question [2] whether there exist solutions of (1) which satisfy $\limsup_{|t|\to\infty} \|u(t)\|_{H^s} = \infty$. Theorem 1 is also motivated by an effective (but not entirely rigorous) statistical description of the cascade toward high frequencies known as *weak turbulence theory* (see for example [4]). The relationship of Theorem 1 to previous literature is discussed in more detail in [3].

We overview the rest of this note and highlight some of the objects appearing in the proof of Theorem 1. Section 2 recasts the *NLS* equation as an equivalent infinite system of ordinary differential equations (ODEs) and introduces a resonant truncation $R\mathscr{F}NLS$ of that ODE system. Section 3 imagines a finite set Λ in the frequency lattice $\mathbb{Z}^2$ satisfying conditions which reduce the resonant truncation $R\mathscr{F}NLS$ to the key object in the proof: the finite dimensional *Toy Model ODE System*. In Sect. 4, the Toy Model System is shown to have a solution with a particular dynamics which drives the cascade of energy toward higher frequencies in *NLS*. Section 5 briefly describes the construction of the special resonant set Λ.

2 NLS as an Infinite System of ODEs

Equation (1) may be gauge transformed into

$$(-i\partial_t + \Delta)v = (G + |v|^2)v \tag{5}$$

by writing $v(t,x) = e^{iGt}u(t,x)$, $G \in \mathbb{R}$. The constant G will soon be chosen to cancel away part of the nonlinearity. Motivated by the explicit solution formula for the linear Schrödinger equation, we make the *ansatz*

$$v(t,x) = \sum_{n\in\mathbb{Z}^2} a_n(t)e^{i(n\cdot x+|n|^2 t)} \tag{6}$$

and the dynamics are recast in terms of the Fourier coefficients $\{a_n(t)\}_{n\in\mathbb{Z}^2}$. A calculation shows that (5) (which is equivalent to (1)) transforms into an infinite ODE system

$$-i\partial_t a_n = Ga_n + \sum_{\substack{n_1,n_2,n_3\in\mathbb{Z}^2\\ n_1-n_2+n_3=n}} a_{n_1}\overline{a_{n_2}}a_{n_3}e^{i\omega_4 t}, \tag{7}$$

where $\omega_4 = |n_1|^2 - |n_2|^2 + |n_3|^2 - |n|^2$. Some manipulations with the sum appearing in (7) and the choice $G = -2\|u(t)\|_{L^2}^2$ cancels away certain nonlinear interactions and recasts (1) into an ODE system ($\mathscr{F}NLS$)

$$-i\partial_t a_n = -a_n|a_n|^2 + \sum_{n_1,n_2,n_3\in\Gamma(n)} a_{n_1}\overline{a_{n_2}}a_{n_3}e^{i\omega_4 t}, \tag{8}$$

where

$$\Gamma(n) = \{(n_1,n_2,n_3)\in(\mathbb{Z}^2)^3 : n_1 - n_2 + n_3 = n, n_1 \neq n, n_3 \neq n\}. \tag{9}$$

The set $\Gamma(n)$ consists of frequency triples which contribute to the dynamics of the Fourier coefficient a_n. Among all triples in $\Gamma(n)$, we expect those in

$$\Gamma_{res}(n) = \{(n_1,n_2,n_3)\in\Gamma(n) : \omega_4 = |n_1|^2 - |n_2|^2 + |n_3|^2 - |n|^2 = 0\}. \tag{10}$$

will have the most influence on the dynamics of a_n. Heuristically, the phase factor $e^{i\omega_4 t}$ oscillates when $\omega_4 \neq 0$ so the time integrated contribution of these nonresonant interactions to a_n should be small compared to those in $\Gamma_{res}(n)$. The defining property for $\Gamma_{res}(n)$ has a geometric interpretation: $(n_1,n_2,n_3)\in\Gamma_{res}(n) \iff (n_1,n_2,n_3,n)$ form four corners of a non-degenerate rectangle with the segment $[n_2,n]$ forming one diagonal and $[n_1,n_3]$ the other.

We define the *resonant truncation* $R\mathscr{F}NLS$ of $\mathscr{F}NLS$ by writing

$$-i\partial_t r_n = -r_n|r_n|^2 + \sum_{(n_1,n_2,n_3)\in\Gamma_{res}(n)} r_{n_1}\overline{r_{n_2}}r_{n_3}. \tag{11}$$

Our proof Theorem 1 constructs initial data $\{r_n(0)\}_{n\in\mathbb{Z}^2}$ such that:

- The evolution $r_n(0) \longmapsto r_n(t)$ satisfying $R\mathscr{F}NLS$ satisfies the conclusions of Theorem 1.
- The evolution $r_n(0) = a_n(0) \longmapsto a_n(t)$ satisfying $\mathscr{F}NLS$ is well-approximated by $r_n(t)$.

The approximation step is standard and involves making the heuristic ideas about the non-resonant interactions rigorous using a non-stationary phase analysis. Building the data $\{r_n(0)\}_{n\in\mathbb{Z}^2}$ which evolves along $R\mathscr{F}NLS$ from low toward high frequencies as in the statement of Theorem 1 is more intricate and is outlined in what follows.

3 Conditions on a Finite Set $\Lambda \subset \mathbb{Z}^2$

The initial data $\{r_n(0)\}_{n\in\mathbb{Z}^2}$ that we construct will satisfy $r_n(0) = 0$ unless $n \in \Lambda \subset \mathbb{Z}^2$ where Λ is a specially designed finite set of lattice points. The set Λ and the data $\{r_n(0)\}$ will be constructed to satisfy a list of conditions which lead to a simplification of $R\mathscr{F}NLS$ which we call the *Toy Model ODE System*.

Imagine we can build a finite set $\Lambda \subset \mathbb{Z}^2$ and choose initial data $\{r_n(0)\}_{n\in\Lambda}$ satisfying the following properties. For some integer N (eventually chosen to depend upon the parameters s, δ, K appearing in Theorem 1), the set Λ breaks up into N disjoint *generations* $\Lambda = \Lambda_1 \cup \cdots \cup \Lambda_N$. Each generation is comprised of nuclear families. A *nuclear family* is a rectangle (n_1, n_2, n_3, n_4) where the frequencies[1] n_1, n_3 (known as the "parents") live in a generation Λ_j, and the frequencies n_2, n_4 (known as the "children") live in the next generation Λ_{j+1}. Suppose further that the following conditions hold true:

1. *Initial Data Support*: The initial data $r_n(0)$ is entirely supported in Λ (i.e. $r_n(0) = 0$ whenever $n \notin \Lambda$).
2. *Closure*: Whenever (n_1, n_2, n_3, n_4) is a rectangle in $\mathbb{Z}^2$ such that three of the corners lie in Λ, then the fourth corner must lie in Λ. In other words, $(n_1, n_2, n_3) \in \Gamma_{res}(n), n_1, n_2, n_3 \in \Lambda \implies n \in \Lambda$.
3. $\exists!$ *Spouse & Children*: $\forall 1 \leq j < N$ and $\forall n_1 \in \Lambda_j$ $\exists$ a unique nuclear family (n_1, n_2, n_3, n_4) (up to trivial permutations) such that n_1 is a parent of this family. In particular each $n_1 \in \Lambda_j$ has a unique spouse $n_3 \in \Lambda_j$ and has two unique children $n_2, n_4 \in \Lambda_{j+1}$.
4. $\exists!$ *Sibling & Parents*: $\forall 1 \leq j < N$ and $\forall n_2 \in \Lambda_{j+1} \exists$ a unique nuclear family (n_1, n_2, n_3, n_4) (up to trivial permutations) such that n_2 is a child of this family. In particular each $n_2 \in \Lambda_{j+1}$ has a unique sibling $n_4 \in \Lambda_{j+1}$ and two unique parents $n_1, n_3 \in \Lambda_j$.
5. *Nondegeneracy*: The sibling of a frequency n is never equal to its spouse.
6. *Faithfulness*: Besides nuclear families, Λ contains no other rectangles.

[1] Note that if (n_1, n_2, n_3, n_4) is a nuclear family, then so is (n_1, n_4, n_3, n_2), (n_3, n_2, n_1, n_4), and (n_3, n_4, n_1, n_2); we shall call these the *trivial permutations* of the nuclear family.

7. *Intragenerational Equality*: The function $n \mapsto r_n(0)$ is constant on each generation Λ_j. Thus $1 \le j \le N$ and $n, n' \in \Lambda_j$ imply $r_n(0) = r_{n'}(0)$.
8. *Norm Explosion*: $\sum_{n\in\Lambda_{N-2}} |n|^{2s} \gtrsim \frac{K^2}{\delta^2} \sum_{n\in\Lambda_3} |n|^{2s}$.
9. *Inner Radius*: For large enough fixed $\mathscr{R}$, $\Lambda \cap \{n \in \mathbb{Z}^2 : |n| < \mathscr{R}\} = \phi$. In other words, Λ is supported far from the frequency origin.

Simple arguments based on the Gronwall inequality show that the initial data support and intragenerational equality conditions propagate under $R\mathscr{F}NLS$. In other words, for all times t, the solution $\{r_n(t)\}_{n\in\mathbb{Z}^2}$ of $R\mathscr{F}NLS$ emerging from data satisfying the conditions above will satisfy $r_n(t) = 0$ for all $n \notin \Lambda$ and $r_n(t) = r_{n'}(t)$ for $n, n' \in \Lambda_j$. Propagation of support implies that $R\mathscr{F}NLS$ collapses to an ODE indexed by $n \in \Lambda$. Propagation of intragenerational equality means that, for each fixed t, the function $n \mapsto r_n(t)$ is constant for $n \in \Lambda_j$. We can therefore introduce $b_j(t) = r_n(t),\ n \in \Lambda_j$ and collapse further to

$$-i\partial_t b_j(t) = -|b_j(t)|^2 b_j(t) + 2b_{j-1}(t)^2\overline{b_j}(t) + 2b_{j+1}(t)^2\overline{b_j}(t), \qquad (12)$$

which we call the *Toy Model ODE System*.

4 Arnold Diffusion for the Toy Model ODE

The system (12) defines a vector flow $t \mapsto \mathbf{b}(t) = \{b_1(t), \ldots, b_N(t)\} \in \mathbb{C}^N$. A calculation shows that $|\mathbf{b}(t)|^2 = \sum_{j=1}^N |b_j(t)|^2 = |\mathbf{b}(0)|^2$. In particular, the unit sphere $\mathbb{S} = \{\mathbf{x} \in \mathbb{C}^N : |\mathbf{x}| = 1\}$ in $\mathbb{C}^N$ is invariant under the Toy Model flow.

Inside the sphere, we have the *coordinate circles* $\mathbb{T}_1, \ldots, \mathbb{T}_N$ defined by $\mathbb{T}_j = \{(b_1, \ldots, b_N) \in \mathbb{S} : |b_j| = 1, b_k = 0\ \forall k \ne j\}$. For each $j \in \{1, \ldots, N\}$, the vector function $b_j(t) = e^{-i(t+\theta)},\ b_k(t) = 0\ \forall k \ne j$ is an *explicit oscillator solution* of (12) that traverses $\mathbb{T}_j$. Here $\theta \in \mathbb{R}$ is an arbitrary phase parameter.

Between $\mathbb{T}_1$ and $\mathbb{T}_2$, we also have an explicit *slider solution* of (12):

$$b_1(t) = \frac{e^{-it}\omega}{\sqrt{1+e^{2\sqrt{3}t}}}; \qquad b_2(t) = \frac{e^{-it}\omega^2}{\sqrt{1+e^{-2\sqrt{3}t}}}; \qquad b_k(t) = 0 \quad \forall k \ne 1, 2,$$

where $\omega = e^{\frac{2\pi i}{3}}$ is a cube root of unity. This solution approaches the coordinate circle $\mathbb{T}_1$ exponentially fast as $t \to -\infty$ and approaches the coordinate circle $\mathbb{T}_2$ as $t \to +\infty$. There are also slider solutions between $\mathbb{T}_j$ and $\mathbb{T}_{j+1}$ for each $j \in \{1, \ldots, N-1\}$.

Using delicate dynamical systems arguments, we jiggle the sliders to construct a solution of (1) which starts near $\mathbb{T}_3$ and, in a finite time, travels very close to $\mathbb{T}_4$. After another finite time, it departs from near $\mathbb{T}_4$ and moves very close to $\mathbb{T}_5$. The solution continues this pattern of riding across jiggled sliders between $\mathbb{T}_j$ and $\mathbb{T}_{j+1}$ until it arrives very close to $\mathbb{T}_{N-2}$. Let $S(t)$ denote the flow map for (12), so $\mathbf{b}(t) = S(t)\mathbf{b}(0)$ solves (12).

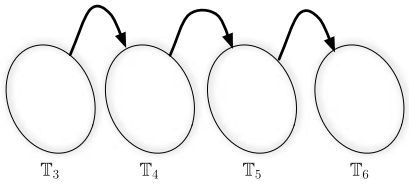

Fig. 1 Explicit oscillator solution around $\mathbb{T}_j$ and the slider solution from $\mathbb{T}_1$ to $\mathbb{T}_2$

Theorem 2 (Arnold Diffusion for (12)). *Let $N \geq 6$. Given any $\epsilon > 0$, there exists a point $\mathbf{x}_3 \in \mathbb{C}^N$ within ϵ of $\mathbb{T}_3$ (using the usual metric on $\mathbb{S}$), a point $\mathbf{x}_{N-2} \in \mathbb{C}^N$ within ϵ of $\mathbb{T}_{N-2}$, and a time $t \geq 0$ such that $S(t)\mathbf{x}_3 = \mathbf{x}_{N-2}$.*

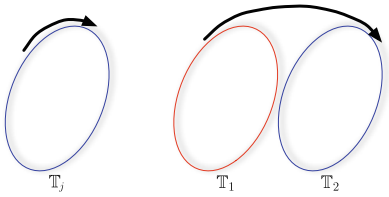

Fig. 2 The idea behind the proof of Theorem 2 is to concatenate jiggled slider solutions to flow from nearby the coordinate circle $\mathbb{T}_3$ to arrive nearby $\mathbb{T}_{N-2}$

We briefly explain how Theorem 2 implies Theorem 1. We can inflate the Toy Model solution of Theorem 2 into a solution of $R\mathscr{F}NLS$ (11) by recalling that $b_j(t) = r_n(t)$, $\forall n \in \Lambda_j$. Thus, this solution of $R\mathscr{F}NLS$ initially starts mostly supported on Λ_3 but evolves to a time when it is mostly supported on Λ_{N-2}. The Norm Explosion condition (8) then implies this solution satisfies the Sobolev norm claims in Theorem 1. Finally, an approximation result, which shows this $R\mathscr{F}NLS$ evolution is appropriately close to the $\mathscr{F}NLS$ (8) evolution emerging from the same data, completes the proof of Theorem 1.

5 Construction of the Resonant Set Λ

We construct a subset Λ of the lattice $\mathbb{Z}^2$ satisfying the eight properties listed in Sect. 3 in two stages. First, we build an abstract *combinatorial model* $\Sigma = \Sigma_1 \cup \cdots \cup \Sigma_N$ which will turn out to be a subset of $\mathbb{C}^{N-1}$. Next, we define a *placement function* $f : \Sigma \to \mathbb{C}$ so that $f(\Sigma) = \Lambda \subset \mathbb{Z}^2$.

We describe the construction of the combinatorial model Σ. We define the *standard unit square* $S \subset \mathbb{C}$ to be the four element set $S = \{0, 1, 1+i, i\}$. We decompose this set $S = S_1 \cup S_2$ where $S_1 = \{1, i\}$ and $S_2 = \{0, 1+i\}$. We define $\Sigma_j \subset \mathbb{C}^{N-1}$ to be the set of all $(N-1)$-tuples $(z_1, \ldots, z_{N-1})$ such that $z_1, \ldots, z_{j-1} \in S_2$ and

$z_j, \ldots, z_{N-1} \in S_1$. Thus, $\Sigma_j = S_2^{j-1} \times S_1^{N-j}$. We define $\Sigma = \Sigma_1 \cup \cdots \cup \Sigma_N$. The set Σ_j is the j^{th} *generation* of Σ.

Consider the four element set $F \subset \Sigma_j \cup \Sigma_{j+1}$ defined by

$$F = \{(z_1, \ldots z_{j-1}, w, z_{j+1}, \ldots, z_N) : w \in S\}$$

where $z_1, \ldots, z_{j-1} \in S_2$ and $z_{j+1}, \ldots, z_N \in S_1$ are all fixed and w varies among the four points of the standard unit square. The two elements of F corresponding to $w \in S_1$, which we denote F_1, F_i, are in generation Σ_j (the parents) while the two elements corresponding to $w \in S_2$, which we denote F_0, F_{1+i}, are in generation Σ_{j+1} (the children). We call the four element set F a *combinatorial nuclear family connecting generations* Σ_j, Σ_{j+1}. For each j, there exists 2^{N-2} combinatorial nuclear families connecting generations Σ_j, Σ_{j+1}. The existence and uniqueness conditions (3), (4) and the nondegeneracy condition (5) can now be checked to hold true for Σ.

Next, we motivate aspects of the construction of the placement function which embeds Σ into a subset of the frequency lattice $\mathbb{Z}^2$. We identify $\mathbb{Z}^2$ with the Gaussian integers $\mathbb{Z}[i]$ in the discussion below. Suppose $f_1 : \Sigma_1 \to \mathbb{C}$ is defined. This means that the frequencies in the first generation have been placed on the plane. We want to define $f_2 : \Sigma_2 \to \mathbb{C}$, that is we want to place down the next generation of frequencies, in such a way that the images of combinatorial nuclear families connecting generations Σ_1, Σ_2 form rectangles in the frequency lattice. We want the combinatorial nuclear families to map to nuclear families linking generations Λ_j, Λ_{j+1}. The diagonal of the rectangle going from two parent frequencies in Λ_1 is determined by f_1. The constraint that the image of the combinatorial nuclear families form rectangles in the plane does not determine the placement of the child frequencies. Indeed, there is the freedom to choose the angle between the diagonals of the rectangle. Therefore, for each $j \in \{1, \ldots, N-1\}$ and for each combinatorial nuclear family F connecting generations Σ_j, Σ_{j+1}, we define an angle $\theta(F) \in \mathbb{R}/2\pi\mathbb{Z}$.

The placement function is then defined recursively with respect to the generation index j using the angles associated to the nuclear families. Suppose that we have defined the placement function components $f_j : \Sigma_j \to \mathbb{C}$ for all $j \in \{1, \ldots, k\}$ for some $k < N - 1$. We need to define $f_{k+1} : \Sigma_{k+1} \to \mathbb{C}$ to set up the recursion. By the combinatorial construction of Σ, each element of Σ_{k+1} is a child of a unique (up to trivial permutations) combinatorial nuclear family linking Σ_k, Σ_{k+1}. We define $f_{k+1} : \Sigma_{k+1} \to \mathbb{C}$ by requiring

$$f_{k+1}(F_{1+i}) = \frac{1 + e^{i\theta(F)}}{2} f_k(F_1) + \frac{1 - e^{i\theta(F)}}{2} f_k(F_i)$$
$$f_{k+1}(F_0) = \frac{1 + e^{i\theta(F)}}{2} f_k(F_1) - \frac{1 - e^{i\theta(F)}}{2} f_k(F_i)$$

for all combinatorial nuclear families F connecting Σ_k, Σ_{k+1}.

Using some measure theory, the density of the complex rationals $\mathbb{Q}[i]$ in $\mathbb{C}$, and the fact that the angles of Pythagorean[2] triangles are dense in $\mathbb{R}/2\pi\mathbb{Z}$, we show that there are choices of the initial placement function f_1 and the angles $\theta(F)$ which define a lattice subset Λ satisfying the required properties:

Theorem 3 (Construction of a good placement function). *Let $N \geq 2$, $s > 1$, and let $\mathscr{R}$ be a sufficiently large integer (depending on N). Then there exists an initial placement function $f_1 : \Sigma_1 \to \mathbb{C}$ and choices of angles $\theta(F)$ for each nuclear family F (and thus an associated complete placement function $f : \Sigma \to \mathbb{C}$) with the following properties:*

- (*Nondegeneracy*) *The function f is injective.*
- (*Integrality*) *We have $f(\Sigma) \subset \mathbb{Z}[i]$.*
- (*Magnitude*) *We have $C(N)^{-1}\mathscr{R} \leq |f(x)| \leq C(N)\mathscr{R}$ for all $x \in \Sigma$.*
- (*Closure and Faithfulness*) *If $x_1, x_2, x_3 \in \Sigma$ are distinct elements of Σ are such that $f(x_1)$, $f(x_2)$, $f(x_3)$ form the three corners of a right-angled triangle, then x_1, x_2, x_3 belong to a combinatorial nuclear family.*
- (*Norm explosion*) *We have*

$$\sum_{n \in f(\Sigma_{N-2})} |n|^{2s} > \frac{1}{2} 2^{(s-1)(N-5)} \sum_{n \in f(\Sigma_3)} |n|^{2s}.$$

The reader is invited to consult [3] for further details.

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[2] Pythagorean triangles are right triangles with integer sides.

Angular Momentum-Mass Inequality for Axisymmetric Black Holes

Sergio Dain

Abstract In these notes we describe recent results concerning the inequality $m \geq \sqrt{|J|}$ for axially symmetric black holes.

1 Introduction

The following conjectures constitute the essence of the current standard picture of the gravitational collapse: (i) Gravitational collapse results in a black hole (weak cosmic censorship) (ii) The spacetime settles down to a stationary final state. If we further assume that at some finite time all the matter fields have fallen into the black hole and hence the exterior region is pure vacuum (for simplicity we discard electromagnetic fields in the exterior), then the black hole uniqueness theorem implies that the final state should be the Kerr black hole. The Kerr black hole is uniquely characterized by its mass m_0 and angular momentum J_0. These quantities satisfy the following remarkable inequality

$$\sqrt{|J_0|} \leq m_0. \tag{1}$$

From Newtonian considerations, we can interpret this inequality as follows[14]: in a collapse the gravitational attraction ($\approx m_0^2/r^2$) at the horizon ($r \approx m_0$) dominates over the centrifugal repulsive forces ($\approx J_0^2/m_0 r^3$).

If the initial conditions for a collapse violate (1) then the extra angular momentum should be radiated away in gravitational waves. However, in an axially symmetric spacetime the angular momentum is a conserved quantity (the Komar integral of the Killing vector, see, for example, [15]). In this case angular momentum cannot be radiated: the angular momentum J of the initial conditions must be equal to the

Sergio Dain
Facultad de Matemática, Astronomía y Física, Universidad Nacional de Córdoba, Ciudad Universitaria, 5000 Córdoba, Argentina, e-mail: name@email.address

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final one J_0. On the other hand, the mass of the initial conditions m satisfies $m \geq m_0$ because gravitational radiation carries positive energy. Then, from inequality (1) we obtain

$$\sqrt{|J|} \leq m. \tag{2}$$

More precisely, (i)–(ii) imply that a complete, vacuum, axisymmetric, asymptotically flat data should satisfy inequality (2), where m and J are the mass and angular momentum of the data. Moreover, the equality in (2) should imply that the data are a slice of extreme Kerr. This is a similar argument to the one used by Penrose [13] to obtain the inequality between mass and the area of the horizon on the initial data. As in the case of Penrose inequality, a counter example of (2) will imply that either (i) or (ii) is not true. Conversely a proof of (2) gives indirect evidence of the validity of (i)–(ii), since it is very hard to understand why this highly nontrivial inequality should hold unless (i)–(ii) can be thought of as providing the underlying physical reason behind it (see the discussion in [16]).

Inequality (2) is a property of the spacetime and not only of the data, since both quantities m and J are independent of the slicing. It is in fact a property of axisymmetric, vacuum, black holes space-times, because a non zero J (in vacuum) implies a non trivial topology on the data and this is expected to signal the presence of a black hole. The physical interpretation of (2) is the following: if we have a stationary vacuum black hole (i.e. Kerr) and add to it axisymmetric gravitational waves, then the spacetime will still have a (non-stationary) black hole, these waves will only increase the mass and not the angular momentum of the spacetime because they are axially symmetric. Since inequality (1) is satisfied for Kerr we get (2).

In this note, we review some recent results (see [10, 5, 9, 6, 7, 4]) in which inequality (2) is proved for one black hole and describe the open problems for the other cases.

2 Variational Principle for the Mass

Inequality (2) suggests the following variational principle:

> *The extreme Kerr initial data are the absolute minimum of the mass among all axisymmetric, vacuum, asymptotically flat and complete initial data with fixed angular momentum.*

However, it is important to note that for two related inequalities, the positive mass theorem and the Penrose inequality, a variational formulation was not successful. In the case of the positive mass theorem only a local version was proved using a variational principle [2].

The key difference in the present case is axial symmetry. As we will see, in that case it possible to write the mass (in an appropriate gauge) as a positive definite integral on a spacelike hypersurface. The reason for this particular behavior of the mass is the following. In the presence of a symmetry, vacuum Einstein equations can be reduced a la Kaluza-Klein to a system on a 3-dimensional manifold where it takes the form of 3-dimensional Einstein equations coupled to a matter source. Since

in 3-dimension there is no radiation (the Weyl tensor is zero), this source represents the true gravitational degree of freedom that have descended from 4-dimensions to appear as "matter" in 3-dimension. Since all the energy is produced by these effective matter sources, one would expect in that, as in other field theories, the total energy of the system can be expressed as a positive definite integral over them. This was in fact proved by Brill [1] in some restricted cases and then generalized in [12, 10, 3]. Using this formula and with the extra assumption that the data are maximal, the variational principle can be formulated in a very simple form [7].

To write the mass formula for axially symmetric spacetimes we follow [8]. Consider a vacuum solution of Einstein's equations, i.e., a four dimensional manifold $\mathscr{V}$ with metric g_{ab} for which the Ricci tensor ${}^{(4)}\mathscr{R}_{ab}$ vanishes. Suppose, in addition, that there exists a spacetime Killing vector η^a. We define the norm and the twist of η^a, respectively, by

$$\lambda^2 = \eta^a \eta^b g_{ab}, \qquad \omega_a = \epsilon_{abcd} \eta^b \bar{\nabla}^c \eta^d, \tag{3}$$

where $\bar{\nabla}_a$ is the connection and ϵ_{abcd} the volume element with respect to g_{ab}. Assuming that the manifold is simply connected and using ${}^{(4)}\mathscr{R}_{ab} = 0$ it is possible to prove that ω_a is the gradient of a scalar field ω

$$\omega_a = \bar{\nabla}_a \omega. \tag{4}$$

In our case the Killing field will be spacelike, i.e. $\lambda \geq 0$.

As we mention above, in the presence of a Killing field, there exists a well known procedure to reduce the field equations [11]. Let $\mathscr{N}$ denote the collection of all trajectories of η^a, and assume that it is a differential 3-manifold. We define the Lorentzian metric h_{ab} on $\mathscr{N}$ by

$$g_{ab} = h_{ab} + \frac{\eta_a \eta_b}{\lambda^2}. \tag{5}$$

Four dimensional Einstein vacuum equation are equivalent to Einstein equations in three dimension on $\mathscr{N}$ coupled to effective matter fields determined by λ and ω. We make a $2+1$ decomposition of these equations. Let n^a be the unit normal vector orthogonal to a spacelike, 2-dimensional slice S. The intrinsic metric on S is denoted by q_{AB} and the trace free part of the second fundamental form of the slice is denoted by k_{AB}. On $(\mathscr{N}, h)$ we fix a gauge: the maximal-isothermal gauge (see [8] for details) and the corresponding coordinates system (t, ρ, z). It is convenient to define the function σ by

$$\lambda = \rho e^{\sigma/2}. \tag{6}$$

In this gauge the mass can be written in the following form

$$m = \frac{1}{16} \int_S \left(2k^{AB} k_{AB} + 3\frac{\lambda'^2}{\lambda^2} + \frac{\omega'^2}{\lambda^4} + |D\sigma|^2 + \frac{|D\omega|^2}{\lambda^4} \right) \rho \, dV_q. \tag{7}$$

where $dV_q = e^{2u} d\rho dz$ denote the volume element with respect to q_{ab}, D is the covariant derivative with respect to q_{AB} with $|D\sigma|^2 = D^A\sigma D_A\sigma$, and the prime denotes directional derivative with respect to n^a, that is

$$\lambda' = n^a \bar{\nabla}_a \lambda. \tag{8}$$

This is essentially a derivative with respect to t. Note that all the terms in the integrand of (7) are positive definite. The first three terms contain the dynamical part of the data, they vanish for stationary solutions, in particular for the Kerr solution. The last two terms, contain the stationary part of the fields. It is important to note that the integral of these terms does not depends on the metric q_{AB}. In effect, the integral of these terms can be written as

$$\mathscr{M}(\sigma, \omega) = \frac{1}{16} \int_{-\infty}^{\infty} dz \int_0^{\infty} d\rho \big(|\partial\sigma|^2 + \rho^{-4} e^{-2\sigma} |\partial\omega|^2 \big) \rho, \tag{9}$$

where ∂ denotes partial derivatives with respect to (ρ, z). The integral (9) depends only on σ and ω. Since we have

$$m \geq \mathscr{M}, \tag{10}$$

to find the minimum of m is equivalent as to find the minimums of $\mathscr{M}$.

In order to write the variational principle, it only remains to discuss the boundary conditions. Physically, we want to prescribe boundary conditions such that the total angular momentum is fixed. The information of the angular momentum is determined by the value of the twist potential ω at the axis $\rho = 0$ (see [7]). To include more than one black hole, we prescribe the following topology. Let i_k be a finite collection of points located at the axis $\rho = 0$. Define the intervals $I_k, 0 \leq k \leq N-1$, to be the open sets in the axis between i_k and i_{k-1}, we also define I_0 and I_N as $z < i_0$ and $z > i_N$ respectively. See Fig. 1. Each point i_k will correspond to an asymptotic end of the data, and hence we will say that the data contain N black holes.

To fix the total angular momentum J (where J is an arbitrary constant) of the data is equivalent as to prescribe the following boundary condition for ω (see [10])

$$\omega|_{I_0} = 4J, \qquad \omega|_{I_N} = -4J. \tag{11}$$

We want to study the minimums of the functional $\mathscr{M}$ with these boundary conditions.

We are now in position to write the precise form of the variational principle.

Conjecture 1. Let σ, ω be arbitrary functions such that ω satisfies the boundary condition (11). Then we have

$$\mathscr{M}(\sigma, \omega) \geq \sqrt{|J|}. \tag{12}$$

Moreover, the equality implies that σ, ω are given by the extreme Kerr solution.

This conjecture was proved for the case $N = 1$ in [10]. This result was extended in [4] to include more generic data.

The conjecture is open for the case $N \geq 2$. For this case, the variational problem is fixed if we impose the boundary condition

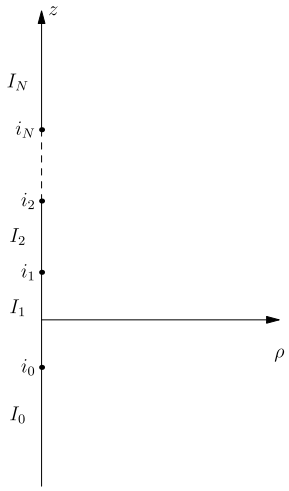

Fig. 1 N asymptotic ends

$$\omega|_{I_i} = 4J_i, \tag{13}$$

with $0 < i < N$, for arbitrary constants J_i. Note however, that conjecture 1 is independent of the values J_i.

Remarkably, in [4] it is proved that the variational problem has a solution (i.e. a minimum) for arbitrary N, but the value of $\mathscr{M}$ for this solution is not known. In order to prove the conjecture for $N \geq 2$, one need to compute a lower bound for this quantity. This problem is related with the uniqueness of the Kerr black hole with degenerate and disconnected horizons.

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Almost Everything About the Fibonacci Operator

David Damanik

Abstract We consider the Fibonacci operator and discuss results that have been obtained for the spectrum, the spectral measures, and the rate of wavepacket spreading. Our presentation is centered around a distortion result that describes the preimage of balls under the trace of the transfer matrix associated with sites given by Fibonacci numbers.

1 Introduction

This paper is concerned with the Fibonacci operator, which is a discrete one-dimensional Schrödinger operator

$$[Hu](n) = u(n+1) + u(n-1) + V(n)u(n) \tag{1}$$

in $\ell^2(\mathbb{Z})$ with potential $V : \mathbb{Z} \to \mathbb{R}$ given by

$$V(n) = \lambda \chi_{[1-\phi,1)}(n\phi + \theta \mod 1). \tag{2}$$

Here, $\lambda > 0$ is the coupling constant, $\phi = \frac{\sqrt{5}-1}{2}$ is the inverse of the golden mean, and $\theta \in [0, 1)$ is the phase. By strong approximation it may be shown that the spectrum of H does not depend on the phase θ. The spectrum of H does, however, depend on the value of the coupling constant λ and we will henceforth denote it by Σ_λ.

The Fibonacci operator plays a prominent role in the context of one-dimensional quasicrystals and it has been studied since the early 1980's in numerous physics and mathematics papers. In this paper, we will focus on the mathematical results that

David Damanik
Department of Mathematics, Rice University, Houston, TX 77005, USA,
e-mail: damanik@rice.edu

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have been obtained for this operator. References to the relevant physics literature can be found, for example, in the review articles [4, 30].

Natural questions concern the location and size of Σ_λ, the type of the spectral measures, and the long-time asymptotics of the solutions to the time-dependent Schrödinger equation, $i\partial_t\psi = H\psi$. Many of these questions have been answered completely, while others have been partially answered. Central to all of these results is the so-called trace map, which is a dynamical system that describes the evolution of the traces of the transfer matrices associated with H along the sequence of Fibonacci numbers.

We describe the trace map and the crucial distortion result in Sect. 2. The location of the spectrum can be described with the help of the trace map. In Sect. 3, we discuss the size of the spectrum as a subset of the real line; namely, it always has zero Lebesgue measure and, for coupling sufficiently large, we give upper and lower bounds on its fractal dimension. These bounds agree in the $\lambda \to \infty$ limit. The spectral measures are always purely singular continuous, as discussed in Sect. 4. We sketch the Gordon two-block method that allows one to exclude eigenvalues for all parameter values. Absence of absolutely continuous spectrum is of course a consequence of zero-measure spectrum. Finally, in Sect. 5, we consider the rate at which an initially localized wavepacket spreads out in space if the time-evolution is given by the unitary group generated by the Fibonacci operator. If the coupling constant is sufficiently large, there are upper and lower bounds for the spreading rate that show behavior which is different from the one that occurs for periodic or random potentials. In other words, the intermediate spectral type is indeed reflected by intermediate wavepacket spreading behavior.

2 The Trace Map

It is useful to rewrite the difference equation

$$u(n+1) + u(n-1) + V(n)u(n) = zu(n) \tag{3}$$

in the form

$$\begin{pmatrix} u(n+1) \\ u(n) \end{pmatrix} = \Phi(n,z) \begin{pmatrix} u(1) \\ u(0) \end{pmatrix}, \tag{4}$$

where the transfer matrices $\Phi(n,z)$ are given by $\Phi(n,z) = T(n,z) \times \cdots \times T(1,z)$ and

$$T(m,z) = \begin{pmatrix} z - V(m) & -1 \\ 1 & 0 \end{pmatrix}.$$

For $z \in \mathbb{C}$ and $k \geq 1$, set $M_k(z) = \Phi(F_k, z)$, where the potential V is given by (2) with $\theta = 0$ and F_k is the k-th Fibonacci number, that is, $F_0 = F_1 = 1$ and $F_{k+1} = F_k + F_{k-1}$ for $k \geq 1$. These matrices obey

$$M_{k+1}(z) = M_{k-1}(z)M_k(z) \tag{5}$$

for $k \geq 2$. For the variables $x_k(z) = \frac{1}{2}\mathrm{Tr}\, M_k(z)$, we have the recursion

$$x_{k+1}(z) = 2x_k(z)x_{k-1}(z) - x_{k-2}(z) \tag{6}$$

and the invariant

$$x_{k+1}(z)^2 + x_k(z)^2 + x_{k-1}(z)^2 - 2x_{k+1}(z)x_k(z)x_{k-1}(z) - 1 \equiv \frac{\lambda^2}{4}. \tag{7}$$

Letting $x_{-1}(z) = 1$ and $x_0(z) = \frac{z}{2}$, the recursion (6) holds for all $k \geq 0$. See, for example, [28] for these results.

The trace map is defined as follows,

$$\mathcal{T} : (x, y, z) \mapsto (2xy - z, x, y),$$

and it may be defined on either $\mathbb{R}^3$ or $\mathbb{C}^3$, depending on the context. The forward orbit of the point $(\frac{z-\lambda}{2}, \frac{z}{2}, 1)$ under the trace map generates the sequence $\{x_k(z)\}$. Namely, for $k \geq 0$, $x_k(z)$ is the second component of $\mathcal{T}^k(\frac{z-\lambda}{2}, \frac{z}{2}, 1)$.

Let $\delta \geq 0$. A necessary and sufficient condition that $x_k(z)$ be unbounded is that

$$|x_{N-1}(z)| \leq 1 + \delta, \quad |x_N(z)| > 1 + \delta, \quad |x_{N+1}(z)| > 1 + \delta \tag{8}$$

for some $N \geq 0$; see [10]. This N is unique. Moreover, in this case we have $|x_{N+k}(z)| \geq (1 + \delta)^{F_k}$ for $k \geq 0$. Thus, it is natural to consider the sets $\sigma_k^\delta = \{z \in \mathbb{C} : |x_k(z)| \leq 1 + \delta\}$, for which we have $\sigma_k^\delta \cup \sigma_{k-1}^\delta \supseteq \sigma_{k+1}^\delta \cup \sigma_k^\delta$. A strong approximation argument then shows that

$$\Sigma_\lambda = \bigcap_k \sigma_{k+1}^\delta \cup \sigma_k^\delta. \tag{9}$$

In particular, $\{x_k(z)\}$ is bounded for every $z \in \Sigma_\lambda$. The invariant (7) yields a λ-dependent upper bound that works uniformly for all such z's.

Moreover, assuming $\lambda > \lambda_0(\delta) = [12(1+\delta)^2+8(1+\delta)^3+4]^{1/2}$, the invariant (7) implies that $\sigma_k^\delta \cap \sigma_{k+1}^\delta \cap \sigma_{k+2}^\delta = \emptyset$ and that the set σ_k^δ has exactly F_k connected components. Each of them is a topological disk that is symmetric about the real axis.

All roots of x_k are real. Consider such a root z and define $\omega(z) = \#\{0 \leq l \leq k-1 : |x_l(z)| \leq 1\}$. Let $c_{k,m} = \#\{\text{roots of } x_k \text{ with } \omega(z) = m\}$. An explicit formula for $c_{k,m}$ was found in [14, Lemma 5] (noting that our $c_{k,m}$ equals $a_{k,m} + b_{k,m}$ in the notation of that paper). In particular, it follows from [14] that, for every $k \geq 2$, $c_{k,m}$ is non-zero if and only if $\frac{k}{2} \leq m \leq \frac{2k}{3}$.

Let $\{z_k^{(j)}\}_{1 \leq j \leq F_k}$ be the roots of x_k and write $\omega_k^{(j)} = \omega(z_k^{(j)})$ for $1 \leq j \leq F_k$. Denote by $B(z, r)$ the open ball in $\mathbb{C}$ that is centered at z and has radius r. Define

$$S_u(\lambda) = 2\lambda + 22 \quad \text{and} \quad S_l(\lambda) = \frac{1}{2}\big((\lambda - 4) + \sqrt{(\lambda - 4)^2 - 12}\big). \tag{10}$$

Then, we have the following distortion result [10, 11].

Theorem 1. *Fix $k \geq 3$, $\delta > 0$, and $\lambda > \max\{\lambda_0(2\delta), 8\}$. Then, there are constants $c_\delta, d_\delta > 0$ such that*

$$\bigcup_{j=1}^{F_k} B\big(z_k^{(j)}, r_k^{(j)}\big) \subseteq \sigma_k^\delta \subseteq \bigcup_{j=1}^{F_k} B\big(z_k^{(j)}, R_k^{(j)}\big), \tag{11}$$

where $r_k^{(j)} = c_\delta S_u(\lambda)^{-\omega_k^{(j)}}$, and $R_k^{(j)} = d_\delta S_l(\lambda)^{-\omega_k^{(j)}}$. The first inclusion in (11) only needs the assumption $\lambda > \lambda_0(2\delta)$.

The proof relies on the Koebe Distortion Theorem and upper and lower bounds for the derivative of x_k at the roots. Such bounds were shown in [8, 22, 27]. We point out that Raymond's paper [27] developed a number of tools that have proved to be useful in the quantitative study of the trace map, some of which have been refined and extended in later papers such as [14, 8, 22].

3 The Cantor Structure and the Dimension of the Spectrum

In this section we discuss properties of the spectrum of the Fibonacci operator as a subset of the real line.

The location of the spectrum can be conveniently described with the help of the trace map; compare (9). While (11) is a useful tool in the study of the size of the spectrum at large values of the coupling constant, there is actually a result that holds for all couplings.

Theorem 2. *For every $\lambda > 0$, the spectrum of the Fibonacci operator has zero Lebesgue measure,* $\mathrm{Leb}(\Sigma_\lambda) = 0$.

Since the spectrum is closed and does not contain any isolated points by general principles, it follows from Theorem 2 that the spectrum of the Fibonacci operator is always a Cantor set.

This result was shown by Sütő in 1989 [29]; see also [1] for a contemporaneous proof by Bellissard, Iochum, Scoppola and Testard of zero measure spectrum for potentials (2) with ϕ replaced by an arbitrary irrational number and a more recent paper by Lenz [25] who develops a completely different approach to zero measure spectrum that is even more general in scope.

Let us describe the main steps in the proof of zero-measure spectrum based on the trace map. The Lyapunov exponent is defined by

$$\gamma(z) = \lim_{n\to\infty} \frac{1}{n} \log \|\Phi(n, z)\|.$$

Here we choose $\theta = 0$ and leave the dependence of $\gamma(z)$ on λ implicit. It was shown by Hof that the limit exists and is the same as the one obtained when one averages over the phase [16]. Consider the set $\mathscr{Z}_\lambda = \{z : \gamma(z) = 0\}$. It follows by general principles that $\mathscr{Z}_\lambda \subseteq \Sigma_\lambda$. In the Fibonacci case, we even have equality. This was shown by Sütő [29] who used the boundedness of $\{x_k(z)\}$ for $z \in \Sigma_\lambda$ to show a subexponential upper bound for $\|\Phi(n, z)\|$. This result was later improved by Iochum and Testard [18] who proved a power-law upper bound for $\|\Phi(n, z)\|$. Both works proved these bounds for the case $\theta = 0$; see [7] for an extension to general θ. On the other hand, Kotani showed in a much more general context (aperiodic ergodic potentials taking finitely many values) that $\mathscr{Z}_\lambda$ has zero Lebesgue measure. Combining these two results, it follows that Σ_λ has zero Lebesgue measure for every $\lambda > 0$.

As a next step, it is natural to study the dimension of the spectrum. Recall that for $S \subseteq \mathbb{R}$ bounded and infinite, the following two dimensions are of interest. For $\alpha \in [0, 1]$, let

$$h^\alpha(S) = \lim_{\delta \to 0} \inf_{\delta-\text{covers}} \sum_{m \geq 1} |I_m|^\alpha$$

and then define the Hausdorff dimension of S by

$$\dim_H(S) = \inf\{\alpha : h^\alpha(S) < \infty\} = \sup\{\alpha : h^\alpha(S) = \infty\}.$$

The lower box counting dimension of S is given by

$$\dim_B^-(S) = \liminf_{\varepsilon \to 0} \frac{\log N_S(\varepsilon)}{\log \frac{1}{\varepsilon}},$$

where $N_S(\varepsilon) = \#\{j \in \mathbb{Z} : [j\varepsilon, (j+1)\varepsilon) \cap S \neq \emptyset\}$. The upper box counting dimension, $\dim_B^+(S)$, is defined with a lim sup in place of the lim inf. When the lower and upper box counting dimensions coincide, we say that the box counting dimension exists and denote it by $\dim_B(S)$.

The following result about these dimensions was obtained for the set Σ_λ in [14].

Theorem 3. *Suppose that $\lambda \geq 16$. Then, the box counting dimension of Σ_λ exists and obeys* $\dim_B(\Sigma_\lambda) = \dim_H(\Sigma_\lambda)$.

The assumption $\lambda \geq 16$ comes from a paper of Casdagli [2], who works under this assumption and proves the hyperbolicity of the trace map, restricted to the invariant surface $\Omega_\lambda = \{(x, y, z) \in \mathbb{R}^3 : x^2 + y^2 + z^2 - 2xyz - 1 = \frac{\lambda^2}{4}\}$; compare (7). It is expected (see [2]) that such a result extends to all $\lambda > 0$. The statement of Theorem 3 then follows from known results for dynamically defined Cantor sets; see [14] for a discussion and references.

In order to describe the large coupling asymptotics of the dimension of the spectrum, let us introduce the function

$$f(x) = \frac{1}{x}\big[(2-3x)\log 2 + (1-x)\log(1-x) \\ - (2x-1)\log(2x-1) - (2-3x)\log(2-3x)\big]$$

on $(\frac{1}{2}, \frac{2}{3})$. f takes its maximum at a unique point $x^* \in (\frac{1}{2}, \frac{2}{3})$. Write $f^* = f(x^*) = \max_{x\in(\frac{1}{2},\frac{2}{3})} f(x)$. Numerics show that $x^* \approx 0.5395$ and $f^* \approx 0.88137$.

Theorem 4. (a) *Suppose* $\lambda > 4$. *Then, we have*

$$\dim_B^-(\Sigma_\lambda) \geq \frac{f^*}{\log S_u(\lambda)}.$$

(b) *Suppose* $\lambda \geq 8$. *Then, we have*

$$\dim_H(\Sigma_\lambda) \leq \frac{f^*}{\log S_l(\lambda)}.$$

Here, $S_u(\lambda)$ and $S_l(\lambda)$ are as defined in (10). As an immediate consequence, we obtain the following exact asymptotic result,

$$\lim_{\lambda\to\infty} \dim(\Sigma_\lambda)\cdot\log\lambda = f^*. \tag{12}$$

We write dim for either $\dim_H$ or $\dim_B$, which is justified by Theorem 3. In particular, this shows that the constant f^* is optimal in both bounds.

The proof of Theorem 4 uses the distortion result described earlier, Theorem 1, along with (9), which links Σ_λ and the sets σ_k^δ. What is needed in addition is a precise result that describes the numbers $\omega_k^{(j)}$. Such a result was obtained in [14], where it is also shown how Theorem 4 then follows from it. It turns out that these coefficients are closely related to the coefficients of the Chebyshev polynomials of the first kind. Since there are explicit formulas for the coefficients of these polynomials, the authors of [14] were able to give explicit formulas for the numbers $\omega_k^{(j)}$. The function f defined above then arises naturally in the limit $k \to \infty$.

There were earlier estimates for the Hausdorff dimension of the spectrum; see Raymond [27] and Liu and Wen [26] (and also [3, 12, 20] for lower bounds obtained indirectly via continuity results for spectral measures). All the bounds behave like a constant times $(\log\lambda)^{-1}$ in the large coupling regime. The earlier papers had weaker constants, whereas the constant f^* found in [14] is optimal as explained above.

4 The Spectral Type

This section will discuss the following result, which determines the spectral type of the Fibonacci operator completely.

Theorem 5. *For every $\lambda > 0$ and every $\theta \in [0, 1)$, the Fibonacci operator has purely singular continuous spectrum.*

One half of the result, the absence of absolutely continuous spectrum, is an immediate consequence of Theorem 2. The set Σ_λ is too small to support an absolutely continuous spectral measure. Historically, however, it was first shown by Kotani that the absolutely continuous spectrum is empty for every $\lambda > 0$ and Lebesgue almost every θ (this is equivalent to $\mathrm{Leb}(\mathscr{Z}_\lambda) = 0$ for every $\lambda > 0$—the result quoted from [23] in the previous section) and the insight contained in Kotani's short paper [23] was the key to all zero measure spectrum results mentioned above [1, 25, 29]. The other half of the result, the absence of eigenvalues, was established in [6] (see [1, 3, 17, 21] for earlier results in this direction).

Let us briefly sketch how eigenvalues, and in fact the existence of decaying solutions to (3) for z's in the spectrum, can be excluded. A crucial realization is that the restriction to the positive half-line of every Fibonacci potential "begins with infinitely many squares". Formally, the result is the following. Choose any $\theta \in [0, 1)$ (and any $\lambda > 0$; we will see that the latter choice is irrelevant for what follows) and consider the transfer matrices $\Phi(n, z)$ associated with the potential (2). Then, for infinitely many values of k, we have that

$$\Phi(2F_k, \cdot) = \Phi(F_k, \cdot)^2. \tag{13}$$

In particular, once such a property holds for one value of $\lambda > 0$, it holds for all values. The subsequence of $\{F_k\}$ for which this statement holds is θ-dependent. The paper [6] develops a partition based approach to Fibonacci potentials from which the result just quoted follows quickly. These partitions are derived from an iteration of the rule (5) and a globalization procedure. In fact, the squares obtained in (13) have the additional property

$$\mathrm{Tr}\, \Phi(F_k, \cdot) = 2x_k(\cdot). \tag{14}$$

By (7) and (9), $|x_k(z)|$ with $z \in \Sigma_\lambda$ and $k \in \mathbb{Z}_+$ is uniformly bounded from above by a constant depending only on λ. Moreover, since transfer matrices always have determinant one, the Cayley-Hamilton Theorem says that

$$\Phi(F_k, z)^2 - (\mathrm{Tr}\, \Phi(F_k, z))\, \Phi(F_k, z) + I = 0. \tag{15}$$

Thus, by (4) and (13)–(15) we see that every non-zero solution u of (3) with $z \in \Sigma_\lambda$ must have $\limsup_{n\to\infty} |u(n)| > 0$. Consequently, there are no decaying (and particularly no ℓ^2) solutions.

The proof sketched here contains three main ideas. The use of the Cayley-Hamilton Theorem to exclude decaying solutions goes back to Gordon [15]. Using the uniform upper bounds for transfer matrix traces to be able to work on a half-line only is an idea of Sütő [28]. The partition approach that allows one to treat all phases was developed by Damanik and Lenz in [6].

5 Bounds on Wavepacket Spreading

In this section we discuss the spreading of an initially localized wavepacket that evolves according to the Schrödinger equation $i\partial_t \psi = H\psi$. We therefore consider $\psi(t) = e^{-itH}\delta_0$ and study its spreading via the time-averaged moments of the position operator,

$$\langle |X|^p_{\delta_0} \rangle (T) = \frac{2}{T} \int_0^\infty e^{-2t/T} \sum_{n\in\mathbb{Z}} |n|^p |\langle e^{-itH}\delta_0, \delta_n \rangle|^2 \, dt,$$

where $p > 0$. To describe the power-law growth of $\langle |X|^p_{\delta_0} \rangle (T)$, consider the lower transport exponent

$$\beta^-_{\delta_0}(p) = \liminf_{T\to\infty} \frac{\log \langle |X|^p_{\delta_0} \rangle (T)}{p \, \log T}$$

and the upper transport exponent

$$\beta^+_{\delta_0}(p) = \limsup_{T\to\infty} \frac{\log \langle |X|^p_{\delta_0} \rangle (T)}{p \, \log T}.$$

Both functions $\beta^\pm_{\delta_0}(p)$ are nondecreasing in p and hence the following limits exist,

$$\alpha^\pm_u = \lim_{p\to\infty} \beta^\pm_{\delta_0}(p).$$

We consider these dynamical quantities for the Fibonacci operator and hence they depend on the parameters λ and θ. The moments grow no faster than $C_\varepsilon T^{p+\varepsilon}$ for any $\varepsilon > 0$ and therefore the transport exponents take values in the interval $[0, 1]$.[1]

There are numerous papers that establish bounds for the spreading of a wavepacket for the Fibonacci operator; see, for example, [3, 11, 8–10, 12–14, 20, 22]. The situation is particularly well understood in the regime of large λ and large p. Here is a result that should be regarded as a companion to Theorem 4.

Theorem 6. (a) *Suppose* $\lambda > \sqrt{24}$. *Then, we have*

$$\alpha^\pm_u \geq \frac{2\log(1+\phi)}{\log S_u(\lambda)}.$$

(b) *Suppose* $\lambda \geq 8$. *Then, we have*

$$\alpha^\pm_u \leq \frac{2\log(1+\phi)}{\log S_l(\lambda)}.$$

[1] As background information, it may be useful to remark that (in the one-dimensional situation we consider here) the transport exponents vanish for random potentials, whereas they are equal to one for periodic potentials. Here we are dealing with a potential of intermediate complexity/disorder and we will see that this is reflected by intermediate transport.

Remarks. (i) These bounds are uniform in θ.

(ii) The functions $S_u(\lambda)$ and $S_l(\lambda)$ are as defined in (10).

(iii) Part (a) is shown in [11], while part (b) is from [10].

(iv) In the limit $\lambda \to \infty$, we find

$$\lim_{\lambda\to\infty} \alpha_u^{\pm} \cdot \log \lambda = 2 \log(1+\phi). \tag{16}$$

The convergence is uniform in θ.

(v) It was shown in [14] that whenever the transfer matrices are bounded by a power law on the spectrum, we have that $\alpha_u^{\pm}$ is bounded from below by the upper/lower box counting dimension of the spectrum. Thus, in the Fibonacci case, we always have

$$\alpha_u^{\pm} \geq \dim_B^{\pm}(\Sigma_\lambda). \tag{17}$$

Comparing (12) and (16), we see that for λ sufficiently large, the inequality (17) is strict.

The papers mentioned above also establish lower bounds for $\beta_{\delta_0}^{\pm}(p)$ for every $\lambda > 0, \theta \in [0, 1)$, and $p > 0$. These bounds show that the transport exponents are always strictly positive. In particular, there is always spreading that is measurable on a power-scale. However, many of these results do not seem to be optimal. This is why (16) is special in this regard as it yields an optimal description of a quantum dynamical quantity in an asymptotic regime. We refer the reader to the original literature for more detailed dynamical lower bounds. As for dynamical upper bounds, Theorem 6(b) is the only known result (see also [5, 22] for earlier weaker results that bound the spreading rate of the slow part of the wavepacket from above). In particular, there are no non-trivial upper bounds for transport exponents for small values of λ and even for $\lambda \geq 8$, there are no upper bounds for $\beta_{\delta_0}^{\pm}(p)$ that improve upon the bound in Theorem 6(b).

Let us describe the mechanisms leading to Theorem 6. The starting point is Kato's formula,

$$\int_0^\infty e^{-2t/T} |\langle e^{-itH}\delta_1, \delta_n\rangle|^2 \, dt = \frac{1}{2\pi} \int_{-\infty}^{\infty} \left|\langle (H - E - \tfrac{i}{T})^{-1}\delta_1, \delta_n\rangle\right|^2 dE$$

which follows quickly from the Plancherel Theorem for the Fourier transform; compare, for example, [22, Lemma 3.2]. This allows one to relate $\langle |X|_{\delta_0}^p \rangle(T)$ to decay properties of the Green function, which in turn is closely related to the growth of the norm of $\Phi(\cdot, E + \frac{i}{T})$. To obtain bounds on the Green function or the norm of the transfer matrix, we start again from the distortion result, Theorem 1. If a complex energy in question, $z = E + \frac{i}{T}$, belongs to a set σ_k^δ, we go "backwards in time" and use (8) to show that up to level k, the traces are bounded by the uniform λ-dependent constant and norms are bounded by a uniform λ-dependent power-law. Conversely, if $z = E + \frac{i}{T}$ does not belong to $\sigma_k^\delta \cup \sigma_{k+1}^\delta$, then the escape condition (8) must have held sometime in the past and by now the trace and hence the norm of the transfer matrix must be very large. Since Theorem 1 allows one to link T and k for such

statements to be true, one can derive explicit bounds for the transfer matrix norm in this way.

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Entanglement-Assisted Quantum Error-Correcting Codes

Igor Devetak, Todd A. Brun and Min-Hsiu Hsieh

Abstract We develop the theory of entanglement-assisted quantum error correcting codes (EAQECCs), a generalization of the stabilizer formalism to the setting in which the sender and receiver have access to pre-shared entanglement. Conventional stabilizer codes are equivalent to self-orthogonal symplectic codes. In contrast, EAQECCs do not require self-orthogonality, which greatly simplifies their construction. We show how any classical quaternary block code can be made into a EAQECC. Furthermore, the error-correcting power of the quantum codes follows directly from the power of the classical codes.

1 Introduction

One of the most important discoveries in quantum information science was the existence of quantum error correcting codes (QECCs) in 1995 [16]. Up to that point, there was a widespread belief that decoherence–environmental noise–would doom any chance of building large scale quantum computers or quantum communication protocols [18], and the equally widespread belief that any analogue of classical error correction was impossible in quantum mechanics. The discovery of quantum

Igor Devetak
Ming Hsieh Electrical Engineering Department, University of Southern California, Los Angeles, CA 90089, USA, e-mail: devetak@usc.edu

Todd A. Brun
Communication Sciences Institute, Department of Electrical Engineering Systems, University of Southern California, 3740 McClintock Ave., EEB 502, Los Angeles, CA 90089-2565 USA, e-mail: tbrun@usc.edu

Min-Hsiu Hsieh
Ming Hsieh Electrical Engineering Department, University of Southern California, Los Angeles, CA 90089, USA, e-mail: minhsiuh@gmail.com

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error correcting codes defied these expectations, and were quickly developed into the theory of stabilizer codes [5, 10]. Moreover, a construction of Calderbank, Shor and Steane [4, 17] showed that it was possible to construct quantum stabilizer codes from classical linear codes–the CSS codes–thereby drawing on the well-studied theory of classical error correction.

Important as these results were, they fell short of doing everything that one might wish. The connection between classical codes and quantum codes was not universal. Rather, only classical codes which satisfied a dual-containing constraint could be used to construct quantum codes. While this constraint was not too difficult to satisfy for relatively small codes, it is a substantial barrier to the use of highly efficient modern codes, such as Turbo codes [1] and Low-Density Parity Check (LDPC) codes [8], in quantum information theory. These codes are capable of achieving the classical capacity; but the difficulty of constructing dual-containing versions of them has made progress toward finding quantum versions very slow.

The results of our entanglement-assisted stabilizer formalism generalize the existing theory of quantum error correction. If the CSS construction for quantum codes is applied to a classical code which is not dual-containing, the resulting "stabilizer" group is not commuting, and thus has no code space. We are able to avoid this problem by making use of pre-existing entanglement. This noncommuting stabilizer group can be embedded in a larger space, which makes the group commute, and allows a code space to be defined. Moreover, this construction can be applied to *any* classical quaternary code, not just dual-containing ones. The existing theory of quantum error correcting codes thus becomes a special case of our theory: dual-containing classical codes give rise to standard quantum codes, while *non-dual-containing classical codes give rise to entanglement-assisted quantum error correction codes* (EAQECCs).

2 Notations

Consider an n-qubit system corresponding to the tensor product Hilbert space $\mathcal{H}_2^{\otimes n}$. Define an n-qubit Pauli matrix $\mathbf{S}$ to be of the form $\mathbf{S} = S_1 \otimes S_2 \otimes \cdots \otimes S_n$, where $S_j \in \{I, X, Y, Z\}$ is an element of the set of Pauli matrices. Let $\mathcal{G}^n$ be the group of all 4^n n-qubit Pauli matrices with all possible phases. Define the equivalence class $[\mathbf{S}] = \{\beta\mathbf{S} \mid \beta \in \mathbb{C}, |\beta| = 1\}$. Then

$$[\mathbf{S}][\mathbf{T}] = [S_1T_1] \otimes [S_2T_2] \otimes \cdots \otimes [S_nT_n] = [\mathbf{ST}].$$

Thus the set $[\mathcal{G}^n] = \{[\mathbf{S}] : \mathbf{S} \in \mathcal{G}^n\}$ is a commutative multiplicative group.

Now consider the group/vector space $(\mathbb{Z}_2)^{2n}$ of binary vectors of length $2n$. Its elements may be written as $\mathbf{u} = (\mathbf{z}|\mathbf{x})$, $\mathbf{z} = z_1 \ldots z_n \in (\mathbb{Z}_2)^n$, $\mathbf{x} = x_1 \ldots x_n \in (\mathbb{Z}_2)^n$. We shall think of $\mathbf{u}$, $\mathbf{z}$ and $\mathbf{x}$ as row vectors. The symplectic product of $\mathbf{u} = (\mathbf{z}|\mathbf{x})$ and $\mathbf{v} = (\mathbf{z}'|\mathbf{x}')$ is given by

$$\mathbf{u} \odot \mathbf{v}^{\mathrm{T}} = \mathbf{z}\,\mathbf{x}'^{\mathrm{T}} + \mathbf{z}'\,\mathbf{x}^{\mathrm{T}}.$$

The right hand side are binary inner products, the superscript T denotes the transpose, and the addition represents Boolean addition.

The map $N : (\mathbb{Z}_2)^{2n} \to \mathcal{G}^n$ is now defined as

$$N_{\mathbf{u}} = N_{u_1} \otimes \cdots \otimes N_{u_n}.$$

Writing

$$X^{\mathbf{x}} = X^{x_1} \otimes \cdots \otimes X^{x_n},$$
$$Z^{\mathbf{z}} = Z^{z_1} \otimes \cdots \otimes Z^{z_n},$$

we have

$$[N_{(\mathbf{z}|\mathbf{x})}] = [Z^{\mathbf{z}} X^{\mathbf{x}}].$$

The two observations hold:

1. The map $[N] : (\mathbb{Z}_2)^{2n} \to [\mathcal{G}^n]$ induced by N is an isomorphism:

$$[N_{\mathbf{u}}][N_{\mathbf{v}}] = [N_{\mathbf{u}+\mathbf{v}}]. \tag{1}$$

2. The commutation relations of the n-qubit Pauli matrices are captured by the symplectic product

$$N_{\mathbf{u}} N_{\mathbf{v}} = (-1)^{\mathbf{u}\odot\mathbf{v}^{\mathrm{T}}} N_{\mathbf{v}} N_{\mathbf{u}}. \tag{2}$$

3 Entanglement-Assisted Quantum Error-Correcting Codes

Denote by $\mathcal{L}$ the space of linear operators defined on the qubit Hilbert space $\mathcal{H}_2$. We will often encounter isometric operators $U : \mathcal{H}_2^{\otimes n_1} \to \mathcal{H}_2^{\otimes n_2}$. The corresponding *superoperator*, or completely positive, trace preserving (CPTP) map, is marked by a hat $\hat{U} : \mathcal{L}^{\otimes n_1} \to \mathcal{L}^{\otimes n_2}$ and defined by

$$\hat{U}(\rho) = U \rho U^{\dagger}.$$

Observe that $\hat{U}$ is independent of any phase factors multiplying U. Thus, for a Pauli operator $N_{\mathbf{u}}$, $\hat{N}_{\mathbf{u}}$ only depends on the equivalence class $[N_{\mathbf{u}}]$.

We consider the following communication scenario depicted in Fig. 1. The protocol involves two spatially separated parties, Alice and Bob, and the resources at their disposal are

- A noisy channel defined by a CPTP map $\mathcal{N} : \mathcal{L}^{\otimes n} \to \mathcal{L}^{\otimes n}$ taking density operators on Alice's system to density operators on Bob's system;
- The c-ebit state $|\Phi\rangle^{\otimes c}$ shared between Alice and Bob.

Alice wishes to send k-qubit quantum information *perfectly* to Bob using the above resources. An $[[n, k; c]]$ entanglement-assisted quantum error-correcting code (EAQECC) consists of

- An encoding isometry $\mathcal{E} = \hat{U}_{\text{enc}} : \mathcal{L}^{\otimes k} \otimes \mathcal{L}^{\otimes c} \to \mathcal{L}^{\otimes n}$
- A decoding CPTP map $\mathcal{D} : \mathcal{L}^{\otimes n} \otimes \mathcal{L}^{\otimes c} \to \mathcal{L}^{\otimes k}$

such that

$$\mathcal{D} \circ \mathcal{N} \circ \hat{U}_{\text{enc}} \circ \hat{U}_{\text{app}} = \text{id}^{\otimes k},$$

where U_{app} is the isometry which appends the state $|\Phi\rangle^{\otimes c}$,

$$U_{\text{app}}|\varphi\rangle = |\varphi\rangle|\Phi\rangle^{\otimes c},$$

and $\text{id} : \mathcal{L} \to \mathcal{L}$ is the identity map on a single qubit. The protocol thus uses up c ebits of entanglement and generates k perfect qubit channels. We represent it by the resource inequality (with a slight abuse of notation [6])

$$\langle \mathcal{N} \rangle + c\,[q\,q] \geq k\,[q \to q].$$

Even though a qubit channel is a strictly stronger resource than its static analogue, an ebit of entanglement, the parameter $k - c$ is still a good (albeit pessimistic) measure of the net noiseless quantum resources gained. It should be borne in mind that a negative value of $k - c$ still refers to a non-trivial protocol.

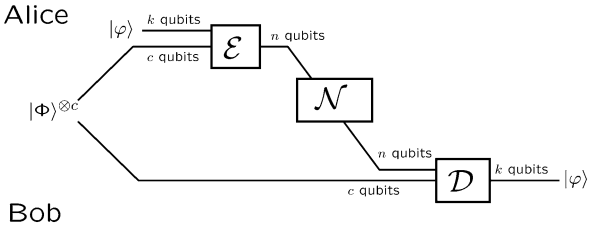

Fig. 1 A generic entanglement assisted quantum code

3.1 The Channel Model: Discretization of Errors

To make contact with classical error correction it is necessary to discretize the errors introduced by $\mathcal{N}$. This is done in two steps. First, the CPTP map $\mathcal{N}$ may be (non-uniquely) written in terms of its Kraus representation

$$\mathcal{N}(\rho) = \sum_i A_i \rho A_i^\dagger.$$

Second, each A_i may be expanded in the Pauli operators

$$A_i = \sum_{\mathbf{u}\in(\mathbb{Z}_2)^{2n}} \alpha_{i,\mathbf{u}} N_{\mathbf{u}}.$$

Define the support of $\mathcal{N}$ by $\mathrm{supp}(\mathcal{N}) = \{\mathbf{u} \in (\mathbb{Z}_2)^{2n} : \exists i, \alpha_{i,\mathbf{u}} \neq 0\}$. The following theorem allows us, absorbing U_{app} into U_{enc}, to replace the continuous map $\mathcal{N}$ by the error set $\mathbf{E} = \mathrm{supp}(\mathcal{N})$.

Theorem 1. *If* $\mathcal{D}\circ\hat{N}_{\mathbf{u}}\circ\hat{U}_{\mathrm{enc}} = \mathrm{id}^{\otimes k}$ *for all* $\mathbf{u} \in \mathrm{supp}(\mathcal{N})$, *then* $\mathcal{D}\circ\mathcal{N}\circ\hat{U}_{\mathrm{enc}} = \mathrm{id}^{\otimes k}$.

Proof. The proof, which follows straightforwardly from the discretization proof in standard QEC case, can be found, e.g. [14]. □

3.2 The Entanglement-Assisted Canonical Code

We can construct the entanglement-assisted canonical code $\mathcal{C}_0^{\mathrm{EA}}$ with the following trivial encoding operation $\mathcal{E}_0 = \hat{U}_0$ defined by

$$U_0 : |\varphi\rangle \to |\underline{0}\rangle \otimes |\Phi\rangle^{\otimes c} \otimes |\varphi\rangle. \tag{3}$$

The operation simply appends ℓ ancilla qubits in the state $|\underline{0}\rangle$, and c copies of $|\Phi\rangle$ (the maximally entangled state shared between sender Alice and receiver Bob), to the initial register containing the state $|\varphi\rangle$ of size k qubits, where $\ell + k + c = n$.

Proposition 2. *The encoding given by* $\mathcal{E}_0$ *and a suitably-defined decoding map* $\mathcal{D}_0$ *can correct the error set*

$$\begin{aligned}\mathbf{E}_0 = \{&X^{\mathbf{a}}Z^{\mathbf{b}} \otimes X^{\mathbf{a}_1}Z^{\mathbf{a}_2} \otimes X^{\alpha(\mathbf{a},\mathbf{a}_1,\mathbf{a}_2)}Z^{\beta(\mathbf{a},\mathbf{a}_1,\mathbf{a}_2)} : \\ &\mathbf{a},\mathbf{b} \in (\mathbb{Z}_2)^{\ell}, \mathbf{a}_1,\mathbf{a}_2 \in (\mathbb{Z}_2)^{c}\},\end{aligned} \tag{4}$$

for any fixed functions $\alpha, \beta : (\mathbb{Z}_2)^{\ell} \times (\mathbb{Z}_2)^{c} \times (\mathbb{Z}_2)^{c} \to (\mathbb{Z}_2)^{k}$.

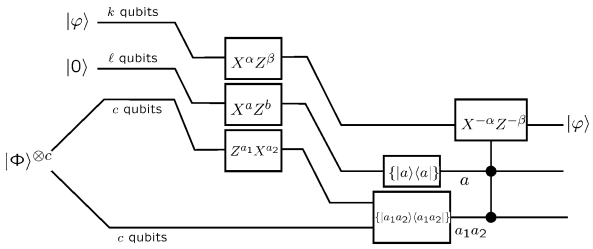

Fig. 2 The canonical code

Proof. The protocol is shown in Fig. 2. After applying an error $E \in \mathbf{E}_0$, the channel output becomes (up to a phase factor):

$$X^{\mathbf{a}}Z^{\mathbf{b}}|\underline{0}\rangle \otimes (X^{\mathbf{a}_1}Z^{\mathbf{a}_2} \otimes I^B)|\Phi\rangle^{\otimes c} \otimes X^{\alpha(\mathbf{a},\mathbf{a}_1,\mathbf{a}_2)}Z^{\beta(\mathbf{a},\mathbf{a}_1,\mathbf{a}_2)}|\varphi\rangle = |\mathbf{a}\rangle \otimes |\mathbf{a}_1,\mathbf{a}_2\rangle \otimes |\varphi'\rangle \tag{5}$$

where

$$\begin{aligned} |\mathbf{a}\rangle &= X^{\mathbf{a}}Z^{\mathbf{b}}|\underline{0}\rangle = X^{\mathbf{a}}|\underline{0}\rangle \\ |\mathbf{a}_1,\mathbf{a}_2\rangle &= (X^{\mathbf{a}_1}Z^{\mathbf{a}_2} \otimes I^B)|\Phi\rangle^{\otimes c} \\ |\varphi'\rangle &= X^{\alpha(\mathbf{a},\mathbf{a}_1,\mathbf{a}_2)}Z^{\beta(\mathbf{a},\mathbf{a}_1,\mathbf{a}_2)}|\varphi\rangle. \end{aligned}$$

As the vector $(\mathbf{a}, \mathbf{a}_1, \mathbf{a}_2, \mathbf{b})$ completely specifies the error E, it is called the *error syndrome*. The state (5) only depends on the *reduced syndrome* $\mathbf{r} = (\mathbf{a}, \mathbf{a}_1, \mathbf{a}_2)$. In effect, $\mathbf{a}$ and $(\mathbf{a}_1, \mathbf{a}_2)$ have been encoded using elementary and superdense coding, respectively. Bob, who holds the entire state (5), can identify the reduced syndrome. Bob simultaneous measures the $Z^{\mathbf{e}_1}, \ldots, Z^{\mathbf{e}_\ell}$ observables to decode $\mathbf{a}$, the $Z^{\mathbf{e}_1} \otimes Z^{\mathbf{e}_1}, \ldots, Z^{\mathbf{e}_c} \otimes Z^{\mathbf{e}_c}$ observables to decode $\mathbf{a}_1$, and the $X^{\mathbf{e}_1} \otimes X^{\mathbf{e}_1}, \ldots, X^{\mathbf{e}_c} \otimes X^{\mathbf{e}_c}$ observables to decode $\mathbf{a}_2$. He then performs $X^{-\alpha(\mathbf{a},\mathbf{a}_1,\mathbf{a}_2)}Z^{-\beta(\mathbf{a},\mathbf{a}_1,\mathbf{a}_2)}$ on the remaining k qubit system $|\varphi'\rangle$, recovering it back to the original state $|\varphi\rangle$.

Since the goal is the transmission of quantum information, no actual measurement is necessary. Instead, Bob can perform the following decoding $\mathcal{D}_0$ consisting of the controlled unitary

$$U_{0,\mathrm{dec}} = \sum_{\mathbf{a},\mathbf{a}_1,\mathbf{a}_2} |\mathbf{a}\rangle\langle\mathbf{a}| \otimes |\mathbf{a}_1,\mathbf{a}_2\rangle\langle\mathbf{a}_1,\mathbf{a}_2| \otimes X^{-\alpha(\mathbf{a},\mathbf{a}_1,\mathbf{a}_2)}Z^{-\beta(\mathbf{a},\mathbf{a}_1,\mathbf{a}_2)}, \tag{6}$$

followed by discarding the unwanted subsystems. □

We can rephrase the above error-correcting procedure in terms of the stabilizer formalism. Let $\mathcal{S}_0 = \langle \mathcal{S}_{0,I}, \mathcal{S}_{0,E} \rangle$, where $\mathcal{S}_{0,I} = \langle Z_1, \ldots, Z_\ell \rangle$ is the isotropic subgroup of size 2^ℓ and $\mathcal{S}_{0,E} = \langle Z_{\ell+1}, \ldots, Z_{\ell+c}, X_{\ell+1}, \ldots, X_{\ell+c} \rangle$ is the *symplectic* subgroup of size 2^{2c}. We can easily construct an Abelian extension of $\mathcal{S}_0$ that acts on $n + c$ qubits, by specifying the following generators:

$$\begin{aligned} &Z_1 \otimes I, \ldots, Z_\ell \otimes I, \\ &Z_{\ell+1} \otimes Z_1, \ldots, Z_{\ell+c} \otimes Z_c, \\ &X_{\ell+1} \otimes X_1, \ldots, X_{\ell+c} \otimes X_c, \end{aligned}$$

where the first n qubits are on the side of the sender (Alice) and the extra c qubits are taken to be on the side of the receiver (Bob). The operators Z_i or X_i to the right of the tensor product symbol above is the Pauli operator Z or X acting on Bob's i-th qubit. We denote such an Abelian extension of the group $\mathcal{S}_0$ by $\widetilde{\mathcal{S}}_0$. It is easy to see that group $\widetilde{\mathcal{S}}_0$ fixes the code space $\mathcal{C}_0^{\mathrm{EA}}$ (therefore $\widetilde{\mathcal{S}}_0$ is the stabilizer for $\mathcal{C}_0^{\mathrm{EA}}$), and we will call the group $\mathcal{S}_0$ the *entanglement-assisted stabilizer* for $\mathcal{C}_0^{\mathrm{EA}}$.

Consider the parameters of the EA canonical code. The number of ancillas ℓ is equal to the number of generators for the isotropic subgroup $\mathcal{S}_{0,I}$. The number of ebits c is equal to the number of symplectic pairs that generate the entanglement subgroup $\mathcal{S}_{0,E}$. Finally, the number of logical qubits k that can be encoded in C_0^{EA}

is equal to $n - \ell - c$. To sum up, C_0^{EA} defined by $\mathcal{S}_0$ is an $[[n, k; c]]$ EAQECC that fixes a 2^k-dimensional code space.

Proposition 3. *The EAQECC C_0^{EA} defined by $\mathcal{S}_0 = \langle \mathcal{S}_{0,I}, \mathcal{S}_{0,E} \rangle$ can correct an error set $\mathbf{E}_0$ if for all $E_1, E_2 \in \mathbf{E}_0$, $E_2^\dagger E_1 \in \mathcal{S}_{0,I} \bigcup (\mathcal{G}_n - \mathcal{Z}(\langle \mathcal{S}_{0,I}, \mathcal{S}_{0,E} \rangle))$.*

Proof. Since the vector $(\mathbf{a}, \mathbf{a}_1, \mathbf{a}_2, \mathbf{b})$ completely specifies the error operator E, we consider the following two different cases:

- If two error operators E_1 and E_2 have the same reduced syndrome $(\mathbf{a}, \mathbf{a}_1, \mathbf{a}_2)$, then the error operator $E_2^\dagger E_1$ gives us all-zero reduced syndrome. Therefore, $E_2^\dagger E_1 \in \mathcal{S}_{0,I}$. This error $E_2^\dagger E_1$ has no effect on the codewords of $\mathcal{C}_0^{\mathrm{EA}}$.
- If two error operators E_1 and E_2 have different reduced syndromes, and let $(\mathbf{a}, \mathbf{a}_1, \mathbf{a}_2)$ be the reduced syndrome of $E_2^\dagger E_1$, then $E_2^\dagger E_1 \notin Z(\langle \mathcal{S}_{0,I}, \mathcal{S}_{0,E} \rangle)$. This error $E_2^\dagger E_1$ can be corrected by the decoding operation given in (6). □

3.3 The General Case

We now present our main result: how to convert an arbitrary subgroup of $\mathcal{G}_n$ into a EAQECC. We need the following two lemmas.

Lemma 4 ([7]). *Let $\mathcal{V}$ be an arbitrary subgroup of $\mathcal{G}_n$ with size 2^m. Then there exists a set of generators $\{\overline{Z}_1, \cdots, \overline{Z}_{p+q}, \overline{X}_{p+1}, \cdots, \overline{X}_{p+q}\}$ that generates $\mathcal{V}$ such that the $\overline{Z}$'s and $\overline{X}$'s obey the same commutation relations as in (7), for some $p, q \geq 0$ and $p + 2q = m$.*

$$\begin{aligned} [\overline{Z}_i, \overline{Z}_j] &= 0 \quad \forall i, j \\ [\overline{X}_i, \overline{X}_j] &= 0 \quad \forall i, j \\ [\overline{X}_i, \overline{Z}_j] &= 0 \quad \forall i \neq j \\ \{\overline{X}_i, \overline{Z}_i\} &= 0 \quad \forall i. \end{aligned} \tag{7}$$

The following lemma is a simply result from group theory, and a proof can be obtained from [3].

Lemma 5. *If there is a one-to-one map between $\mathcal{V}$ and $\mathcal{S}$ which preserves their commutation relations, which we denote $\mathcal{V} \sim \mathcal{S}$, then there exists a unitary U such that for each $V_i \in \mathcal{V}$, there is a corresponding $S_i \in \mathcal{S}$ such that $V_i = U S_i U^{-1}$, up to a phase which can differ for each generator.*

We our now ready for our main result:

Theorem 6. *Given a general group $\mathcal{S} = \langle \mathcal{S}_I, \mathcal{S}_E \rangle$ with the sizes of $\mathcal{S}_I$ and $\mathcal{S}_E$ being 2^{n-k-c} and 2^{2c}, respectively, there exists an $[[n, k; c]]$ EAQECC $\mathcal{C}^{EA}$ defined by the encoding and decoding pair $(\mathcal{E}, \mathcal{D})$ with the following properties:*

1. *The code* $\mathcal{C}^{EA}$ *can correct the error set* $\mathbf{E}$ *if for all* $E_1, E_2 \in \mathbf{E}$, $E_2^\dagger E_1 \in \mathcal{S}_I \cup (\mathcal{G}_n - \mathcal{Z}(\langle \mathcal{S}_I, \mathcal{S}_E \rangle))$.
2. *The codespace* $\mathcal{C}^{EA}$ *is a simultaneous eigenspace of the Abelian extension of* $\mathcal{S}$.
3. *To decode, the reduced error syndrome is obtained by simultaneously measuring the observables from* $\widetilde{\mathcal{S}}$.

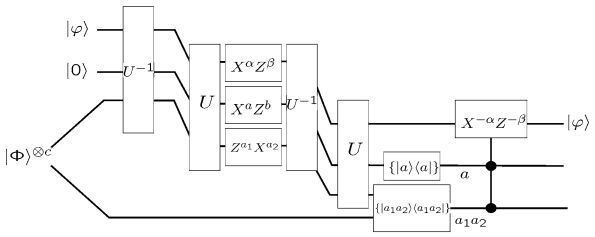

Fig. 3 Generalizing the canonical code construction

Proof. Since the commutation relations of $\mathcal{S}$ are the same as the EA stabilizer $\mathcal{S}_0$ for the EA canonical code $\mathcal{C}_0^{\mathrm{EA}}$ in the previous section, by Lemma 5, there exists an unitary matrix U such that $\mathcal{S}_0 = U\mathcal{S}U^{-1}$. Define $\mathcal{E} = U^{-1} \circ \mathcal{E}_0$ and $\mathcal{D} = \mathcal{D}_0 \circ \hat{U}$, where $\hat{U}$ is the trivial extension of U are Bob's Hilbert space, and $\mathcal{E}_0$ and $\mathcal{D}_0$ are given in (3) and (6), respectively.

1. Since
$$\mathcal{D}_0 \circ E_0 \circ \mathcal{E}_0 = \mathrm{id}^{\otimes k}$$
for any $E_0 \in \mathbf{E}_0$, then
$$\mathcal{D} \circ E \circ \mathcal{E} = \mathrm{id}^{\otimes k}$$
follows for any $E \in \mathbf{E}$. Thus, the encoding and decoding pair $(\mathcal{E}, \mathcal{D})$ corrects $\mathbf{E}$.
2. Since $\mathcal{C}_0^{\mathrm{EA}}$ is the simultaneous $+1$ eigenspace of $\widetilde{\mathcal{S}}_0$, $\mathcal{S} = U^{-1}\mathcal{S}_0 U$, and by definition $\mathcal{C}^{\mathrm{EA}} = \hat{U}^{-1}(\mathcal{C}_0^{\mathrm{EA}})$, we conclude that $\mathcal{C}^{\mathrm{EA}}$ is a simultaneous eigenspace of $\widetilde{\mathcal{S}}$.
3. The decoding operation $\mathcal{D}_0$ involves
   i. measuring the set of generators of $\widetilde{\mathcal{S}}_0$, yielding the error syndrome according to the error E_0.
   ii. performing a recovering operation E_0 again to undo the error.

   By Lemma 7, performing $\mathcal{D} = \mathcal{D}_0 \circ \hat{U}$ is equivalent to measuring $\widetilde{\mathcal{S}} = U^{-1}\widetilde{\mathcal{S}}_0 U$, followed by performing the recovering operation UE_0U^{-1} based on the measurement outcome, followed by $\hat{U}$ to undo the encoding. □

Lemma 7. *Performing* U *followed by measuring the operator* $\mathbf{A}$ *is equivalent to measuring the operator* $U^{-1}\mathbf{A}U$ *followed by performing* U.

Proof. Let Π_i be a projector onto the eigenspace corresponding to eigenvalue λ_i of $\mathbf{A}$. Performing U followed by measuring the operator $\mathbf{A}$ is equivalent to the instrument (generalized measurement) given by the set of operators $\{\Pi_i U\}$. The operator $U^{-1}\mathbf{A}U$ has the same eigenvalues as $\mathbf{A}$, and the projector onto the eigenspace

corresponding to eigenvalue λ_i is $U^{-1}\Pi_i U$. Measuring the operator $U^{-1}\mathbf{A}U$ followed by performing U is equivalent to the instrument $\{U(U^{-1}\Pi_i U)\} = \{\Pi_i U\}$. □

3.4 Distance

The notion of distance provides a convenient way to characterize the error correcting properties of a code. We start by defining the *weight* of a vector $\mathbf{u} = (\mathbf{z}|\mathbf{x}) \in (\mathbb{Z}_2)^{2n}$ by $\mathrm{wt}(\mathbf{u}) = \mathrm{wt}(\mathbf{z} \vee \mathbf{x})$. Here $\vee$ denotes the bitwise logical "or", and $\mathrm{wt}(\mathbf{y})$ is the number of non-zero bits in $\mathbf{y} \in (\mathbb{Z}_2)^n$. In terms of the Pauli group, $\mathrm{wt}(\mathbf{u})$ is the number of single qubit Pauli matrices in $N_{\mathbf{u}}$ not equal to the identity I.

A code is said to correct t errors if it corrects the error set $\{\mathbf{u} : \mathrm{wt}(\mathbf{u}) \leq t\}$ but not $\{\mathbf{u} : \mathrm{wt}(\mathbf{u}) \leq t + 1\}$. A code with distance $d = 2t + 1$ can correct t errors. An $[[n, k; c]]$ EAQEC code with distance d will be referred to as an $[[n, k, d; c]]$ code.

3.5 Generalized $\mathbb{F}_4$ Construction

The following Proposition generalizes a result from [5].

Proposition 8. *If a classical* $[n, k, d]_4$ *code exists then an* $[[n, 2k - n + c, d; c]]$ *EAQECC exists for some non-negative integer c.*

Proof. Consider a classical $[n, k, d]_4$ code (the subscript 4 emphasizes that the code is over $\mathbb{F}_4$) with an $(n - k) \times n$ quaternary parity check matrix H_4. By definition, for each nonzero $\mathbf{a} \in (\mathbb{F}_4)^n$ such that $\mathrm{wt}_4(\mathbf{a}) < d$,

$$\langle H_4, \mathbf{a}\rangle \neq \mathbf{0}^{\mathrm{T}}.$$

This is equivalent to the logical statement

$$\mathrm{Tr}\langle \omega H_4, \mathbf{a}\rangle \neq \mathbf{0}^{\mathrm{T}} \vee \mathrm{Tr}\langle \overline{\omega} H_4, \mathbf{a}\rangle \neq \mathbf{0}^{\mathrm{T}}.$$

This is further equivalent to

$$\mathrm{Tr}\langle \widetilde{H}_4, \mathbf{a}\rangle \neq \mathbf{0}^{\mathrm{T}},$$

where

$$\widetilde{H}_4 = \begin{pmatrix} \omega H_4 \\ \overline{\omega} H_4 \end{pmatrix}. \tag{8}$$

Applying the following map between the Pauli operators and elements of $\mathbb{F}_4$, the field with four elements:

Π	I	X	Y	Z
$\mathbb{F}_4$	0	$\overline{\omega}$	1	ω

to $\widetilde{H}_4$ gives us a set of generators for the group $\mathcal{S}$ of some $[[n, 2k - n + c; c]]$ EAQECC by Theorem 6. □

Any classical binary $[n, k, d]_2$ code may be viewed as a quaternary $[n, k, d]_4$ code. In this case, the above construction gives rise to a CSS-type code.

3.6 Bounds on Performance

In this section we shall see that the performance of EAQECCs is comparable to the performance of QECCs (which are a special case of EAQECCs).

The two most important outer bounds for QECCs are the quantum Singleton bound [12, 15] and the quantum Hamming bound [9]. Given an $[[n, k, d]]$ QECC (which is an $[[n, k, d; 0]]$ EAQECC), the quantum Singleton bound reads

$$n - k \geq 2(d - 1).$$

The quantum Hamming bound holds only for non-degenerate codes and reads

$$\sum_{j=0}^{\lfloor \frac{d-1}{2} \rfloor} 3^j \binom{n}{j} \leq 2^{n-k}.$$

The proofs of these bounds [9, 15] are easily adapted to EAQECCs. This was first noted by Bowen [2] in the case of the quantum Hamming bound. Consequently, an $[[n, k, d; c]]$ EAQECC satisfies both bounds for any value of c. Note that the $\mathbb{F}_4$ construction connects the quantum Singleton bound to the classical Singleton bound $n - k \geq d - 1$. An $[n, k, d]_4$ code saturating the classical Singleton bound implies an $[[n, 2k - n + c, d; c]]$ EAQECC saturating the quantum Singleton bound.

It is instructive to examine the asymptotic performance of quantum codes on a particular channel. A popular choice is the tensor power channel $\mathcal{N}^{\otimes n}$, where $\mathcal{N}$ is the depolarizing channel with Kraus operators $\{\sqrt{p_0}I, \sqrt{p_1}X, \sqrt{p_2}Y, \sqrt{p_3}Z\}$, for some probability vector $\mathbf{p} = (p_0, p_1, p_2, p_3)$.

It is well known that the maximal transmission rate $R = k/n$ achievable by a non-degenerate QECC (in the sense of vanishing error for large n on the channel $\mathcal{N}^{\otimes n}$) is equal to the *hashing bound* $R = 1 - H(\mathbf{p})$. Here $H(\mathbf{p})$ is the Shannon entropy of the probability distribution $\mathbf{p}$. This bound is attained by picking a random self-orthogonal code. However no explicit constructions are known which achieve this bound.

Interestingly, the $\mathbb{F}_4$ construction also connects the hashing bound to the Shannon bound for quaternary channels. Consider the quaternary channel $a \mapsto a + c$, where c takes on values $0, \omega, 1, \overline{\omega}$, with respective probabilities p_0, p_1, p_2, p_3. The maximal achievable rate $R = k/n$ for this channel was proved by Shannon to equal $R = 2 - H(\mathbf{p})$. An $[n, k]_4$ code saturating the Shannon bound implies an $[[n, 2k - n + c; c]]$ EAQECC, achieving the hashing bound!

4 Conclusions

A practical advantage of EAQEC codes over standard QEC codes is that they are much easier to construct from classical codes because self-orthogonality is not required. This allows us to import the classical theory of error correction wholesale, including capacity-achieving modern codes. The appeal of these modern codes comes from the existence of efficient decoding algorithms that provide an excellent trade-off between decoding complexity and decoding performance. In fact, these decoding algorithms, such as sum-product algorithm, can be modified to decode the error syndromes effectively [13]. The only problem of using these iterative decoding algorithms on quantum LDPC actually comes from those shortest 4 cycles that were introduced inevitably because of the self-orthogonality constraint. However, by allowing assisted entanglement, those 4 cycles can be eliminated completely, and the performance of the iterative decoding improves substantially in our numerical simulations [11]. This finding further confirms the contribution of our EA formalism. We plan to further examine the performance of classical LDPC codes and turbo codes in the context of the catalyst size for EAQEC codes.

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Particle Decay in Ising Field Theory with Magnetic Field

Gesualdo Delfino

Abstract The scaling limit of the two-dimensional Ising model in the plane of temperature and magnetic field defines a field theory which provides the simplest illustration of non-trivial phenomena such as spontaneous symmetry breaking and confinement. Here we discuss how Ising field theory also gives the simplest model for particle decay. The decay widths computed in this theory provide the obvious test ground for the numerical methods designed to study unstable particles in quantum field theories discretized on a lattice.

1 Ising Field Theory

Quantum field theory provides the natural tool for the characterization of universality classes of critical behavior in statistical mechanics. While the general ideas based on the renormalization group apply to any dimension (see e.g. [2]), the two-dimensional case acquired in the last decades a very special status. Indeed, after the exact description of critical points was made possible by the solution of conformal field theories [1], it appeared that also specific directions in the scaling region of two-dimensional statistical systems can be described exactly [22, 21]. Additional insight then comes from perturbation theory around these integrable directions [8].

The two-dimensional Ising model plays a basic role in the theory of critical phenomena since when Onsager computed its free energy and provided the first exact description of a second order phase transition [17]. Its scaling limit in the plane of temperature and magnetic field defines a field theory—the Ising field theory—which provides the simplest example of non-trivial phenomena such as spontaneous symmetry breaking and confinement [16]. Here we will discuss how Ising field theory also yields the simplest model for particle decay [10].

Gesualdo Delfino
International School for Advanced Studies (SISSA), via Beirut 2-4, 34014 Trieste, Italy and Istituto Nazionale di Fisica Nucleare, Sezione di Trieste, Italy, e-mail: delfino@sissa.it

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The Ising model is defined on a lattice by the reduced Hamiltonian

$$E = -\frac{1}{T}\sum_{\langle i,j\rangle}\sigma_i\sigma_j - H\sum_i \sigma_i, \quad \sigma_i = \pm 1 \tag{1}$$

so that the partition function is $Z = \sum_{\{\sigma_i\}} e^{-E}$. On a regular lattice in more than one dimension, the model undergoes, for a critical value T_c of the temperature and for vanishing magnetic field H, a second order phase transition associated to the spontaneous breakdown of spin reversal symmetry.

In two dimensions the scaling limit of (1) is described by the Ising field theory with action

$$\mathscr{A} = \mathscr{A}_{CFT} - \tau\int d^2x\,\varepsilon(x) - h\int d^2x\,\sigma(x). \tag{2}$$

Here $\mathscr{A}_{CFT}$ is the action of the simplest reflection-positive conformal field theory in two dimensions, which corresponds to the Ising critical point [1]. The spin operator $\sigma(x)$ with scaling dimension $X_\sigma = 1/8$ and the energy operator $\varepsilon(x)$ with scaling dimension $X_\varepsilon = 1$ are, together with the identity, the only relevant operators present in this conformal theory. The couplings h and τ account for the magnetic field and the deviation from critical temperature, respectively.

The field theory (2) describes a family of renormalization group trajectories flowing out of the critical point located at $h = \tau = 0$ (Fig. 1). Since the coupling conjugated to an operator Φ has the dimension of a mass to the power $2 - X_\Phi$, the combination

$$\eta = \frac{\tau}{|h|^{8/15}} \tag{3}$$

is dimensionless and can be used to label the trajectories. In particular, the low- and high-temperature phases at $h = 0$ and the critical isotherm $\tau = 0$ correspond to $\eta = -\infty, +\infty, 0$, respectively.

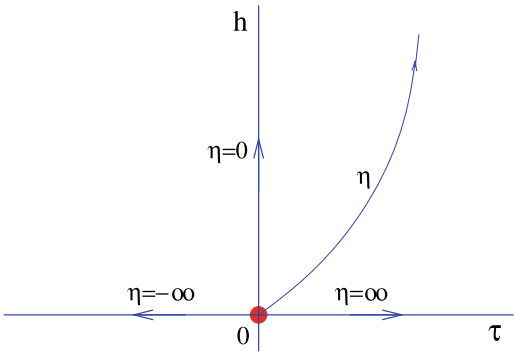

Fig. 1 The Ising field theory (2) describes a one-parameter family of renormalization group trajectories (labelled by η) flowing out of the critical point located at $\tau = h = 0$

2 Evolution of the Mass Spectrum

Under analytic continuation to imaginary time the euclidean field theory (2) defines a $(1+1)$-dimensional relativistic theory allowing for a particle interpretation.

It is well known that the action (2) with $h = 0$ describes a free neutral fermion with mass $m \sim |\tau|$. While in the disordered phase $\tau > 0$ this fermionic particle corresponds to ordinary spin excitations, in the spontaneously broken phase $\tau < 0$ it describes the kinks interpolating between the two degenerate ground states of the system (Fig. 2a). In the euclidean interpretation the space-time trajectories of the kinks correspond to the domain walls separating regions with opposite magnetization.

A small magnetic field switched on at $\tau < 0$ breaks explicitly the spin reversal symmetry and removes the degeneracy of the two ground states (Fig. 2b). To first order in h the energy density difference between the two vacua is

$$\Delta\mathscr{E} \simeq 2h\langle\sigma\rangle, \tag{4}$$

where $\langle\sigma\rangle$ is the spontaneous magnetization at $\tau = 0$. With the symmetry broken the kinks are no longer stable excitations. An antikink-kink pair, which was a two-particle asymptotic state of the theory at $h = 0$, now encloses a region where the system sits on the false vacuum (Fig. 2b). The need to minimize this region induces an attractive potential

$$V(R) \simeq \Delta\mathscr{E}\, R \tag{5}$$

(R is the distance between the walls) which confines the kinks and leaves in the spectrum of the theory only a string of antikink-kink bound states $A_n, n = 1, 2, \ldots,$ whose masses

$$m_n = 2m + \frac{(\Delta\mathscr{E})^{2/3} z_n}{m^{1/3}}, \quad h \to 0 \tag{6}$$

are obtained from the Schrödinger equation with the potential (5). The z_n in (6) are positive numbers determined by the zeros of the Airy function, $\mathrm{Ai}(-z_n) = 0$. This non-relativistic approximation is exact in the limit $h \to 0$ in which $m_n - 2m \to 0$. The spectrum (6) was first obtained in [16] from the study of the analytic structure in momentum space of the spin-spin correlation function for small magnetic field. Relativistic corrections to (6) have been obtained more recently[1] in [23].

The particles A_n with mass larger than twice the lightest mass m_1 are unstable. It was conjectured in [16] that the number of stable particles decreases as η increases from $-\infty$, until only A_1 is left in the spectrum of asymptotic particles as $\eta \to +\infty$. The particle A_1 would then be the free fermion of the theory at $\eta = +\infty$. According to this scenario, for any $n > 1$ there should exist a value η_n for which m_n crosses the decay threshold $2m_1$, so that the particle A_n becomes unstable for $\eta > \eta_n$. The natural expectation is that the values η_n decrease as n increases, in such a way that the τ-h plane is divided into sectors with a different number of stable particles as

[1] See also [24] which appeared after this talk was given.

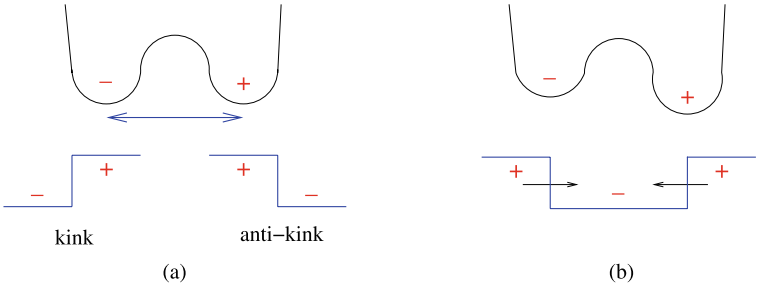

Fig. 2 The free energy and the kink excitations in the spontaneously broken phase (a). A small magnetic field removes the degeneracy of the ground states and confines the kinks (b)

qualitatively shown in Fig. 3. The trajectories corresponding to the values η_n are expected to densely fill the plane in the limit $\eta \to -\infty$.

This pattern has been confirmed by numerical investigations of the spectrum of the field theory (2) for all values of η [8, 23, 24]. For $\eta \to -\infty$ the particles A_n with n large can be studied within the semiclassical approximation and their decay widths have been obtained in [19, 24].

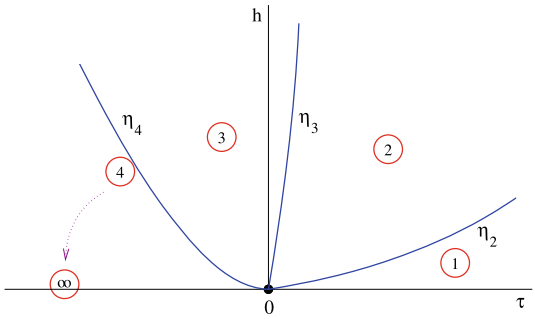

Fig. 3 Expected evolution of the mass spectrum as a function of η. In the sector in between η_n and η_{n+1} the theory possesses n stable particles (numbers in the circles)

3 Particle Decay off the Critical Isotherm

The critical isotherm $\eta = \tau = 0$ must lie within the sector in which the theory has, generically, three stable particles (Fig. 3). To understand this we must recall that A. Zamolodchikov showed in [22, 21] that the theory (2) with $\tau = 0$ is integrable and computed its exact S-matrix. He found that the spectrum along this integrable trajectory consists of eight stable particles $A_1, \ldots, A_8$ with masses

$$
\begin{aligned}
m_1 &\sim h^{8/15} \\
m_2 &= 2m_1 \cos\frac{\pi}{5} = (1.6180339887..)\, m_1 \\
m_3 &= 2m_1 \cos\frac{\pi}{30} = (1.9890437907..)\, m_1 \\
m_4 &= 2m_2 \cos\frac{7\pi}{30} = (2.4048671724..)\, m_1 \\
m_5 &= 2m_2 \cos\frac{2\pi}{15} = (2.9562952015..)\, m_1 \\
m_6 &= 2m_2 \cos\frac{\pi}{30} = (3.2183404585..)\, m_1 \\
m_7 &= 4m_2 \cos\frac{\pi}{5}\cos\frac{7\pi}{30} = (3.8911568233..)\, m_1 \\
m_8 &= 4m_2 \cos\frac{\pi}{5}\cos\frac{2\pi}{15} = (4.7833861168..)\, m_1 .
\end{aligned}
\tag{7}
$$

A peculiarity of this spectrum is that only the lightest three particles lie below the lowest decay threshold $2m_1$. The remaining five have the phase space to decay and certainly are not prevented to do so by internal symmetries (the magnetic field leaves no internal symmetry in the Ising model). It is easy to see that, while there is nothing wrong with the stability of the particles above threshold along this integrable trajectory, they must necessarily decay as soon as a deviation, however small, from the critical temperature breaks integrability [10]. Figure 4 shows the bound state poles and the unitarity cuts of the elastic scattering amplitudes S_{11} and S_{12} in the complex plane of the relativistic invariant s (square of the center of mass energy). We know from [22, 21] that at $\tau = 0$ the scattering channel A_1A_1 produces the first three particles as bound states (Fig. 4a), while the channel A_1A_2 produces the first four (Fig. 4b). The absence of inelastic scattering in integrable theories allows only for the unitarity cut associated to the elastic processes. When integrability is broken (i.e. as soon as we move away from $\tau = 0$), however, the inelastic channels and the associated unitarity cuts open up. In particular, the process $A_1A_2 \to A_1A_1$ acquires a non-zero amplitude, so that the threshold located at $s = 4m_1^2$ becomes the lowest one also in the A_1A_2 scattering channel (Fig. 4c). Since the pole associated to A_4 is located above this threshold, it can no longer remain on the real axis, which in that region is now occupied by the new cut. The position of the pole must then develop an imaginary part which, according to the general requirements for unstable particles [11], is negative and brings the pole through the cut onto the unphysical region of the Riemann surface. The other particles above threshold, which appear as bound states in other amplitudes at $\tau = 0$, decay through a similar mechanism. We see then that, because of integrability, the trajectory $\eta = 0$ corresponds to an isolated case with eight stable particles inside a range of values of η in which only the particles A_1, A_2, A_3 are stable.

These decay processes associated to integrability breaking can be studied analytically through the form factor perturbation theory around integrable models [8]. Indeed, if the action of the perturbed integrable theory is

$$\mathscr{A}_{\text{integrable}} + \lambda \int d^2x\, \Psi(x), \tag{8}$$

the perturbative series in λ can be expressed in terms of the matrix elements of the perturbing operator Ψ on the asymptotic particle states (Fig. 5). These matrix elements can be computed exactly in the unperturbed, integrable theory exploiting analyticity constraints [14, 20] supplemented by operator-dependent asymptotic conditions at high energies [5, 9, 6].

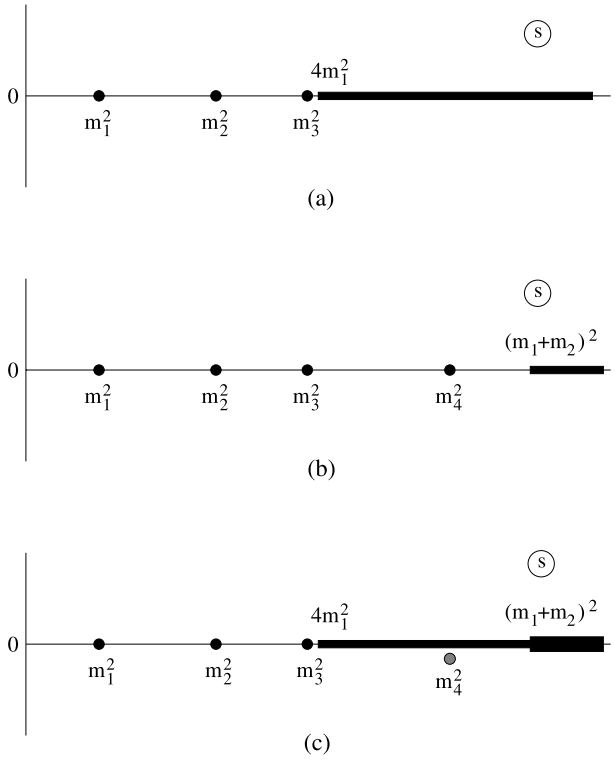

Fig. 4 Poles and unitarity cuts for the elastic scattering amplitudes S_{11} and S_{12} in the integrable case $\tau = 0$, (a) and (b), respectively, and for τ slightly different from zero (c). In (c) the particle A_4 became unstable and the associated pole moved through the cut into the unphysical region

For our present purposes we then look at the action (2) as the integrable trajectory $\tau = 0$ perturbed by the energy operator $\varepsilon(x)$ and must compute corrections in τ. The matrix elements of an operator $\Phi(x)$ in the unperturbed theory can all be related to the form factors[2]

[2] The energy and momentum of the particles are parameterized in terms of rapidities as $(p^0, p^1) = (m_a \cosh\theta, m_a \sinh\theta)$.

$$F^{\Phi}_{a_1\ldots a_n}(\theta_1,\ldots,\theta_n) = \langle 0|\Phi(0)|A_{a_1}(\theta_1)\ldots A_{a_n}(\theta_n)\rangle, \tag{9}$$

where $|0\rangle$ is the vacuum state and the asymptotic states are built in terms of the eight particles which are stable at $\tau = 0$.

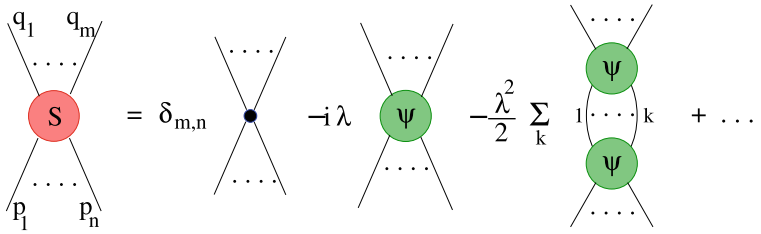

Fig. 5 Perturbative expansion for a scattering amplitude in the theory (8). The matrix elements of the perturbing operator Ψ can be computed exactly in the unperturbed, integrable theory

To lowest order in τ the corrections to the real and imaginary parts of the masses come from the perturbative terms in Fig. 6 and are given by [8]

$$\delta\,\mathrm{Re}\,m_c^2 \simeq -2\tau\ f_c, \tag{10}$$

$$\mathrm{Im}\,m_c^2 \simeq -\tau^2 \sum_{a\le b,\ m_a+m_b\le m_c} 2^{1-\delta_{ab}}\ \frac{|f_{cab}|^2}{m_c m_a|\sinh\theta_a^{(cab)}|}, \quad c = 4, 5 \tag{11}$$

with

$$f_c = F^{\varepsilon}_{cc}(i\pi, 0), \tag{12}$$

$$f_{cab} = F^{\varepsilon}_{cab}(i\pi, \theta_a^{(cab)}, \theta_b^{(cab)}); \tag{13}$$

$\theta_a^{(cab)}$ is determined by energy-momentum conservation at the vertices in Fig. 6b.

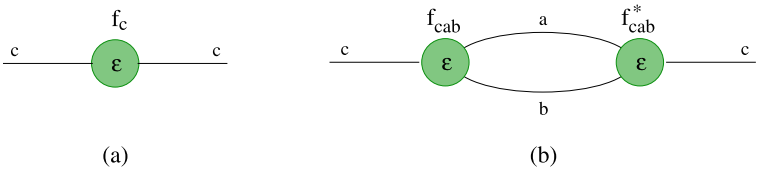

Fig. 6 Terms determining the leading corrections to the real (a) and imaginary (b) parts of the masses in Ising field theory at small τ. For $c > 5$ also diagrams with more than two particles in the intermediate state contribute to the imaginary part

The available decay channels for the particles above threshold are determined by the spectrum (7):

$$
\begin{aligned}
&A_4 \to A_1 A_1 \\
&A_5 \to A_1 A_1, \quad A_1 A_2 \\
&A_6 \to A_1 A_1, \quad A_1 A_2, \quad A_1 A_3, \quad A_1 A_1 A_1,
\end{aligned}
$$

and similarly for A_7 and A_8. For $c > 5$ the sum in (11) must be completed including the contributions of the decay channels with more than two particles in the final state.

One- and two-particle form factors for Ising field theory at $\tau = 0$ have been computed in [5, 7] (see [4] for a review). Table 1 contains the complete list of one-particle matrix elements for the relevant operators. The results for the lightest particle are compared in Table 2 with the result of numerical diagonalization of the transfer matrix on the lattice [3]. Three-particle form factors have been computed in [10] in order to determine the imaginary parts (11).

Table 1 One-particle form factors for the operators σ and ε in Ising field theory at $\tau = 0$ [5, 7]. The rescaling implied by the notation $\hat{\Phi} \equiv \Phi/\langle\Phi\rangle$ ensures that the results in the table are universal

	$\hat{\sigma}$	$\hat{\varepsilon}$
F_1	−0.640902..	−3.706584..
F_2	0.338674..	3.422288..
F_3	−0.186628..	−2.384334..
F_4	0.142771..	2.268406..
F_5	0.060326..	1.213383..
F_6	−0.043389..	−0.961764..
F_7	0.016425..	0.452303..
F_8	−0.003036..	−0.105848..

Table 2 Lightest-particle form factors at $\tau = 0$ from integrable quantum field theory [5, 7] and from numerical diagonalization of the transfer matrix [3]

	Field theory	Lattice
$F_1^{\hat{\sigma}}$	−0.640902..	−0.6408(3)
$F_1^{\hat{\varepsilon}}$	−3.70658..	−3.707(7)

The available results relevant for the leading mass corrections are

$$
\begin{aligned}
f_1 &= (-17.8933..)\langle\varepsilon\rangle \qquad |f_{411}| = (36.73044..)|\langle\varepsilon\rangle| \\
f_2 &= (-24.9467..)\langle\varepsilon\rangle \qquad |f_{511}| = (19.16275..)|\langle\varepsilon\rangle| \\
f_3 &= (-53.6799..)\langle\varepsilon\rangle \qquad |f_{512}| = (11.2183..)|\langle\varepsilon\rangle| \\
f_4 &= (-49.3206..)\langle\varepsilon\rangle
\end{aligned}
$$

where $\langle\varepsilon\rangle$ is taken at $\tau = 0$. The ratios

$$
\lim_{\eta\to 0} \frac{\delta \operatorname{Re} m_a^2}{\delta \mathscr{E}} = 2\,\frac{f_a}{\langle\varepsilon\rangle}, \tag{14}
$$

where $\delta\mathscr{E}$ is the variation of the vacuum energy density, are completely universal and particularly easy to check numerically. These predictions for the variations of the real part of the masses of the first four particles have been confirmed numerically both in the continuum [8, 24] and on the lattice [13]. Using the result[3] [12]

$$\langle\varepsilon\rangle = -(2.00314..)|h|^{8/15}, \tag{15}$$

it easy to check that the sign of the variations

$$\delta r_a = -\frac{\tau f_1}{m_1 m_a}\left(r_a^2 - \frac{f_a}{f_1}\right) + O(\tau^2) \tag{16}$$

of the mass ratios $r_a = \mathrm{Re}\, m_a/m_1$ agrees with the McCoy-Wu scenario (Fig. 7).

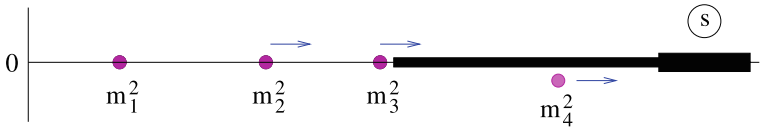

Fig. 7 Evolution of the mass spectrum as predicted by (16) as τ increases from 0. A_2 and A_3 approach the threshold and will decay for positive values of τ; A_4 has already become unstable for $\tau < 0$ and moves further away from the threshold

The above values of f_{abc} give [10]

$$\mathrm{Im}\, m_4^2 \simeq (-173.747..)\tau^2, \tag{17}$$

$$\mathrm{Im}\, m_5^2 \simeq (-49.8217..)\tau^2, \tag{18}$$

and in turn the decay widths and lifetimes

$$\Gamma_a = -\frac{\mathrm{Im}\, m_a^2}{m_a}, \qquad t_a = \frac{1}{\Gamma_a} \tag{19}$$

of the particles A_4 and A_5. The lifetime ratio

$$\lim_{\tau\to 0}\frac{t_4}{t_5} = 0.23326.. \tag{20}$$

is universal, as well as the branching ratio for A_5, which decays at 47% into A_1A_1 and for the remaining fraction into A_1A_2.

It appears from (20) that A_5 lives more than four times longer than A_4, somehow in contrast with the expectation inherited from accelerator physics that, in absence of symmetry obstructions, heavier particles decay more rapidly. Notice, however, that in d dimensions the width for the decay $A_c \to A_aA_b$ is

[3] The value (15) refers to the normalization of ε in which $\langle\varepsilon(x)\varepsilon(0)\rangle \to |x|^{-2}$ as $|x| \to 0$.

$$\Gamma_{c\to ab} \propto g^2 |f_{abc}|^2 \Phi_d, \tag{21}$$

where g is the perturbative parameter, f_{abc} the form factor and

$$\Phi_d \sim \int \frac{d^{d-1}\mathbf{p}_a}{p_a^0} \frac{d^{d-1}\mathbf{p}_b}{p_b^0} \delta^d(p_a + p_b - p_c) \sim \frac{|\mathbf{p}|^{d-3}}{m_c} \tag{22}$$

the phase space ($\mathbf{p} = \mathbf{p}_a = -\mathbf{p}_b$). For fixed decay products, $|\mathbf{p}|$ increases with m_c and in $d = 2$ suppresses the phase space, in contrast with what happens in $d = 4$. The results for the vertices f_{abc} indicate that in our case the dynamics further enhances the increase of t_c with m_c.

4 Unstable Particles in Finite Volume

The issue of obtaining numerical checks of theoretical predictions for decay processes is made particularly interesting by the difficulty of characterizing unstable particles in the finite volume [15]. The problem is particularly relevant for lattice gauge theories.

In two dimensions energy spectra can be obtained by numerical diagonalization of a truncated Hamiltonian on a cylinder geometry. The signature of particle decay on the cylinder is clear. At an integrable point, when the energy levels are plotted as a function of the circumference R of the cylinder, the line corresponding to a particle above threshold crosses infinitely many levels which belong to the continuum when $R = \infty$ (Fig. 8). Once integrability is broken, this line "disappears" through a removal of level crossings and a reshaping of the lines associated to stable excitations (Fig. 9).

One way of extracting the decay width from such a spectrum is the following [15]. Consider energy levels corresponding to states with two particles of mass m and momenta p and $-p$, sufficiently close to the threshold $E = 2m$ that the particles can only scatter elastically, with scattering amplitude $S(p) = \exp i\delta(p)$. On the circle, p is quantized by the condition $e^{iRp} S(p) = 1$, or equivalently

$$Rp + \delta(p) = 2\pi n, \tag{23}$$

with n labelling the states. Hence $\delta(p)$ can be determined from the measure of

$$E(R) = 2\sqrt{p^2 + m^2}. \tag{24}$$

A narrow resonance of mass m_c and width Γ can then be fitted through the Breit-Wigner formula

$$\delta(p) = \delta_0(p) + \delta_{BW}(p), \qquad \delta_{BW} = -i \ln \frac{E - m_c - i\Gamma/2}{E - m_c + i\Gamma/2}, \tag{25}$$

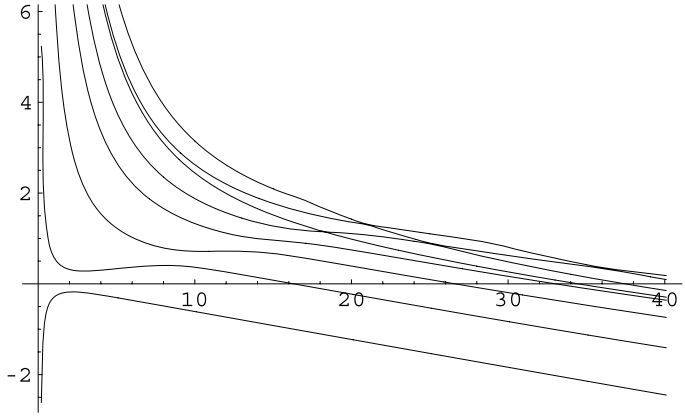

Fig. 8 First eight energy levels of the finite volume Hamiltonian of Ising field theory at $\tau = 0$ as functions of $r = m_1 R$ (from Ref. [8]). At $r = 40$, starting from the bottom, the levels are identified as the ground state, the first three particle states A_1, A_2 and A_3, three scattering states $A_1 A_1$, the particle above threshold A_4. Crossings between the line associated to the latter and the scattering states are visible around $r = 18$, $r = 25$ and $r = 36$

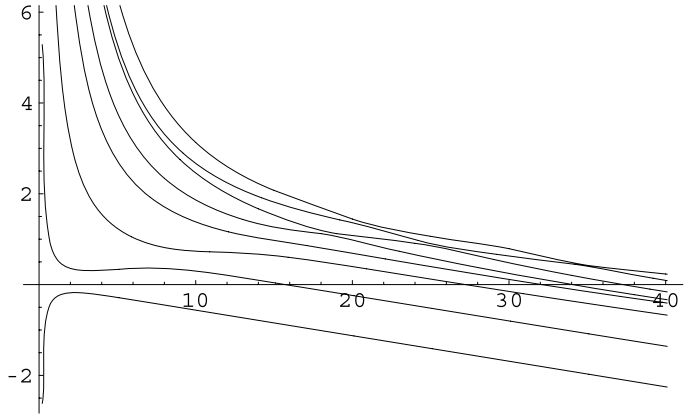

Fig. 9 First eight energy levels of the finite volume Hamiltonian of Ising field theory slightly away from $\tau = 0$ (from Ref. [8]). Observe the splitting of the crossings pointed out in the previous figure

δ_0 being a smooth background.

An alternative method was proposed in [10]. At an integrable point consider a particle with mass $m_c > m_a + m_b$. The states

$$|A_c(p = 0)\rangle \equiv |1\rangle, \qquad |A_a(p)A_b(-p)\rangle \equiv |2\rangle \tag{26}$$

are degenerate on the cylinder at a crossing point R^*. When integrability is broken by a perturbation

$$V = \lambda \int_0^R dx \Psi(x), \tag{27}$$

the energy splitting at R^* is, to lowest order in perturbation theory,

$$\Delta E = \sqrt{(V_{11} - V_{22})^2 + 4|V_{12}|^2}, \tag{28}$$

where $V_{ij} = \langle i|V|j\rangle$. Choosing a crossing point at R^* large enough, the V_{ij}'s are well approximated by the infinite volume matrix elements. In this way the decay vertices V_{12} can be obtained from measures of the energy splittings.

Both methods have been used in [18] to measure the decay widths of the first two particles above threshold in Ising field theory close to the critical temperature. The results are shown in Table 3 together with the predictions of form factor perturbation theory discussed in the previous section. It seems obvious that any numerical method designed to measure decay widths in more complicated lattice models should first of all be able to recover these predictions for the two-dimensional Ising model.

Table 3 The values of the three-particle vertices $\hat{f}_{abc} \equiv f_{abc}/\langle\varepsilon\rangle$ obtained numerically in [18] compared with the exact predictions of [10]

$\lvert\hat{f}_{cab}\rvert$	Exact	Numerical
$\lvert\hat{f}_{411}\rvert$	36.730..	36.5(3)
$\lvert\hat{f}_{511}\rvert$	19.163..	19.5(9)

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Fluctuations and Large Deviations in Non-equilibrium Systems

Bernard Derrida

Abstract For systems in contact with two reservoirs at different densities, the large deviation function of the density gives a possible way of extending the notion of free energy to non-equilibrium systems. This large deviation function of the density can be calculated explicitly for exclusion models in one dimension with open boundary conditions. For the simple exclusion process as well as for other diffusive systems, one can also obtain the distribution of the current of particles flowing through the system and the results lead to a simple conjecture for the large deviation function of the current of more general diffusive systems.

1 Introduction

The goal of the talk was to give a short review on results [6, 13–18, 20] obtained over the last few years on systems maintained in a non-equilibrium steady state by contact with two or more heat baths at unequal temperatures or with several reservoirs at unequal densities.

Let us first consider a system in contact with two heat baths at temperatures T_a and T_b as in Fig. 1.

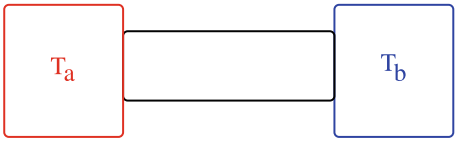

Fig. 1 A system in contact with two heat baths at temperatures T_a and T_b

Bernard Derrida
Laboratoire de Physique Statistique, Ecole Normale Supérieure, 24 rue Lhomond, 75231 Paris Cedex 05, France, e-mail: derrida@lps.ens.fr

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When $T_a = T_b = T$, i.e. when the system is at equilibrium, one knows from equilibrium statistical mechanics that each microscopic configuration $\mathscr{C}$ of energy $E(\mathscr{C})$ is occupied according to its Boltzmann weight

$$P_{\text{equilibrium}}(C) = Z^{-1} \exp\left[-\frac{E(C)}{kT}\right]. \tag{1}$$

One can then define the free energy

$$F = -T \log Z = -T \log\left(\sum_{\mathscr{C}} \exp\left[-\frac{E(\mathscr{C})}{T}\right]\right) \tag{2}$$

from which macroscopic properties such as the average energy or the specific heat can be obtained.

When $T_a \neq T_b$, the system reaches in the long time limit a steady state, but there is no longer a general expression such as (1) for the steady state probabilities of microscopic configurations

$$P_{\text{non-equilibrium}}(C) = ?$$

and there is no a priori definition of the free energy. One of the first questions one may ask is to know what $P_{\text{non-equilibrium}}(C)$ looks like and how the notion of free energy can be extended to non-equilibrium systems. New questions also arise related to the flow of energy Q_t through the system during a time interval t, i.e. the energy Q_t transferred from one reservoir to the other or equivalently the entropy production $Q_t(\frac{1}{T_b} - \frac{1}{T_a})$. One can for example try to determine the probability distribution $P(Q_t)$ of this energy flux.

Another non-equilibrium steady state situation one may consider is that of a system exchanging particles with two reservoirs at densities ρ_a and ρ_b. When $\rho_a \neq \rho_b$ (and in absence of external field) there is a flow of particles through the system. One can then ask the same questions as before: for example what is the average current of particles between the two reservoirs, what is the density profile through the system, what are the fluctuations or the large deviations of this current or of the density.

2 Large Deviation Function of the Density

One way of extending the notion of free energy to non-equilibrium systems is to define the large deviation function [28] of the density. For a box of volume V containing Vr particles, the probability $P_v(n)$ of finding n particles in a subvolume v has the following large n and v dependence

$$P_v(n) \sim \exp\left[-va\left(\frac{n}{v}\right)\right] \tag{3}$$

where $a(\rho)$ is the large deviation function at density ρ. Figure 2 shows a typical shape of $a(\rho)$ for a homogeneous system (i.e. not at a coexistence between different phases) with a single minimum at $\rho = r$ where $a(r) = 0$.

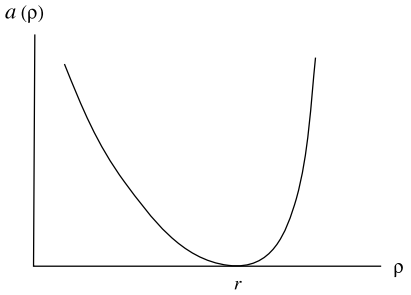

Fig. 2 A typical shape of the large deviation function $a(\rho)$ of the density

The large deviation function $a(\rho)$ can be defined for equilibrium systems as well as for non-equilibrium systems. For equilibrium systems, it is closely related to the free energy: if the volume v is sufficiently large and if the interactions are short ranged, the large deviation function $a(\rho)$ is given by

$$a(\rho) = \frac{f(\rho) - f(r) - (\rho - r) f'(r)}{kT} \tag{4}$$

where $f(\rho)$ is the free energy per unit volume. This can be seen by noticing that for $v \ll V$ and when $v^{1/d}$ is much larger that the range of the interactions

$$P_v(n) = \frac{Z_v(n) Z_{V-v}(N-n)}{Z_V(N)} \exp\left[O\left(v^{\frac{d-1}{d}}\right)\right] \tag{5}$$

where the term $\exp[O(v^{\frac{d-1}{d}})]$ represents the interactions between pairs of particles, one of which is the volume v and the other one in $V - v$. Then taking the log of (5) and using the fact that

$$\lim_{v \to \infty} \frac{\log Z_v(v\rho)}{v} = -\frac{f(\rho)}{kT} \tag{6}$$

leads to (4).

3 Free Energy Functional

If one divides a system of linear size L into n boxes of linear size l (in dimension d, one has $n = L^d / l^d$ such boxes), one can try to determine the probability of finding a certain density profile $\{\rho_1, \rho_2, \ldots, \rho_n\}$, i.e. the probability of seeing $l^d \rho_1$ particles in the first box, $l^d \rho_2$ particles in the second box, $\ldots$ $l^d \rho_n$ in the nth box. For large L

one expects the following L dependence of this probability

$$\mathrm{Pro}(\rho_1, \ldots, \rho_n) \sim \exp\left[-L^d \mathscr{F}(\rho_1, \rho_2, \ldots, \rho_n)\right] \tag{7}$$

where $\mathscr{F}$ is a large deviation function which generalizes $a(\rho)$ introduced in (3). If

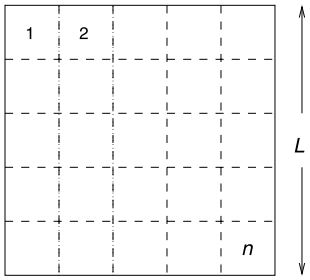

Fig. 3 One specifies the density ρ_i in each box i

one defines a reduced coordinate $\mathbf{x}$ by

$$\mathbf{r} = L\mathbf{x} \tag{8}$$

and if one takes the limit $l \to \infty$ with $l \ll L$ so that the number of boxes becomes infinite, one gets a functional $\mathscr{F}(\rho(\mathbf{x}))$ for an arbitrary density profile $\rho(\mathbf{x})$

$$\mathrm{Pro}(\rho(\mathbf{x})) \sim \exp\left[-L^d \mathscr{F}(\rho(\mathbf{x}))\right]. \tag{9}$$

At equilibrium the functional $\mathscr{F}$ can be expressed in terms of the free energy $f(\rho)$ per unit volume (6) at density ρ: for a system of Vr particles with short range pair interactions in a volume $V = L^d$, one has

$$\mathrm{Pro}(\rho_1, \ldots, \rho_n) = \frac{Z_v(v\rho_1) \ldots Z_v(v\rho_n)}{Z_V(Vr)} \exp\left[O\left(\frac{L^d}{l}\right)\right] \tag{10}$$

where $v = l^d$. Comparing with (7), in the limit $L \to \infty$, $l \to \infty$, keeping n fixed gives

$$\mathscr{F}(\rho_1, \rho_2, \ldots, \rho_n) = \frac{1}{kT} \frac{1}{n} \sum_{i=1}^{n} [f(\rho_i) - f(r)]. \tag{11}$$

In the limit of an infinite number of boxes, this becomes

$$\mathscr{F}(\rho(\mathbf{x})) = \frac{1}{kT} \int d\mathbf{x} [f(\rho(\mathbf{x})) - f(r)]. \tag{12}$$

Thus, *at equilibrium*, the large deviation functional $\mathscr{F}$ is fully determined by the knowledge of the free energy $f(\rho)$ per unit volume and one knows that

- $\mathscr{F}$ is a *local* functional of $\rho(\mathbf{x})$ (see (12)).
- It is also *convex* (as the free energy $f(\rho)$ is a convex function of ρ).
- By expanding (12) around the most likely profile $\overline{\rho}(\mathbf{x}) = r$, one obtains also from (12) that *the fluctuations of the density profile are Gaussian* with a variance related to the second derivative of the free energy, i.e. related to the compressibility as predicted by Smoluchowski and Einstein.
- One knows (by the Landau argument) that, with short range interactions, there is no phase transition in one dimension.

For *non-equilibrium* systems, the large deviation functional of the density has been calculated so far in very few cases [2, 5, 10, 13–16, 20]. In these exactly solvable cases, one finds that

- The large deviation function is in general *non-local* (see for example its expressions for the simple exclusion process SSEP in Sect. 5). This non-locality is directly related to the presence of *long range correlations* (see Sect. 9).
- In some cases such as the asymmetric simple exclusion process ASEP, the functional is *non-convex* [15, 16].
- It also happens that for the ASEP, *the fluctuations of the density are sometimes non-Gaussian* [15, 16, 18] and are not related to the expansion of the functional around the most likely profile.
- It is also well known that non-equilibrium systems may exhibit *phase transitions in one dimension* [10–12, 21, 26, 29, 33].

4 Simple Exclusion Processes (SSEP)

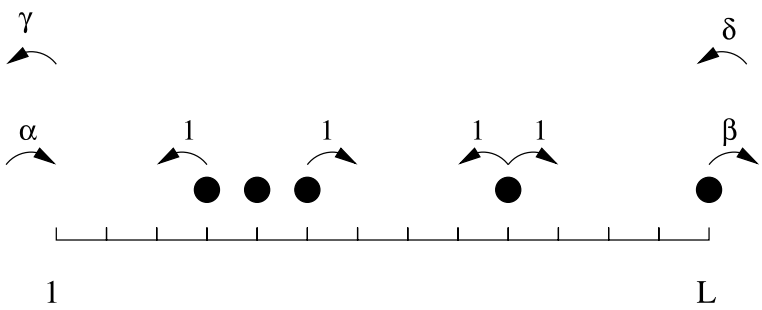

Fig. 4 The symmetric simple exclusion process

One of the simplest cases for which the large deviation functions $a(\rho)$ or $\mathscr{F}(\rho(x))$ can be calculated is the symmetric simple exclusion process [9, 32, 35] shown in Fig. 4. The model is defined as a one dimensional lattice of L sites with open boundaries, each site being either empty or occupied by a single particle. During every infinitesimal time interval dt, each particle has a probability dt of jumping

to the left if the neighboring site on its left is empty, dt of jumping to the right if the neighboring site on its right is empty. At the two boundaries the dynamics is modified to mimic the coupling with reservoirs of particles: at the left boundary, during each time interval dt, a particle is injected on site 1 with probability αdt (if this site is empty) and a particle is removed from site 1 with probability γdt (if this site is occupied). Similarly on site L, particles are injected at rate δ and removed at rate β.

One can show [13, 14, 20] that these choices of the rates $\alpha, \gamma, \beta, \delta$ correspond to the left boundary being connected to a reservoir at density ρ_a and the right boundary to a reservoir at density ρ_b with ρ_a and ρ_b given by

$$\rho_a = \frac{\alpha}{\alpha+\gamma}; \qquad \rho_b = \frac{\delta}{\beta+\delta}. \tag{13}$$

For the SSEP, it is easy to determine the steady state profile: if $\tau_i = 0$ or 1 is a binary variable indicating whether site i is empty or occupied, the time evolution of the average occupation $\langle \tau_i \rangle$ is given by

$$\begin{aligned} \frac{d\langle \tau_1 \rangle}{dt} &= \alpha - (\alpha+\gamma+1)\langle \tau_1 \rangle + \langle \tau_2 \rangle \\ \frac{d\langle \tau_i \rangle}{dt} &= \langle \tau_{i-1} \rangle - 2\langle \tau_i \rangle + \langle \tau_{i+1} \rangle \quad \text{for } 2 \le i \le L-1 \\ \frac{d\langle \tau_L \rangle}{dt} &= \langle \tau_{L-1} \rangle - (1+\beta+\delta)\langle \tau_L \rangle + \delta \end{aligned} \tag{14}$$

and the steady state density profile (obtained by writing that $\frac{d\langle \tau_i \rangle}{dt} = 0$) is

$$\langle \tau_i \rangle = \frac{\rho_a(L + \frac{1}{\beta+\delta} - i) + \rho_b(i - 1 + \frac{1}{\alpha+\gamma})}{L + \frac{1}{\alpha+\gamma} + \frac{1}{\beta+\delta} - 1}. \tag{15}$$

The average current

$$\langle J \rangle = \langle \tau_i - \tau_{i+1} \rangle = \frac{\rho_a - \rho_b}{L + \frac{1}{\alpha+\gamma} + \frac{1}{\beta+\delta} - 1} \simeq \frac{\rho_a - \rho_b}{L} \tag{16}$$

is proportional to the gradient of the density (with a coefficient of proportionality which is here simply 1) and therefore follows Fick's law.

One can write down the equations which generalize (14) and govern the time evolution of the two-point function or higher correlations. For example one finds [19, 34] in the steady state for $1 \le i < j \le L$

$$\begin{aligned} \langle \tau_i \tau_j \rangle_c &\equiv \langle \tau_i \tau_j \rangle - \langle \tau_i \rangle \langle \tau_j \rangle \\ &= -\frac{(\frac{1}{\alpha+\gamma} + i - 1)(\frac{1}{\beta+\delta} + L - j)}{(\frac{1}{\alpha+\gamma} + \frac{1}{\beta+\delta} + L - 1)^2 (\frac{1}{\alpha+\gamma} + \frac{1}{\beta+\delta} + L - 2)} (\rho_a - \rho_b)^2. \end{aligned} \tag{17}$$

For large L, if one introduces macroscopic coordinates $i = Lx$ and $j = Ly$, this becomes for $x < y$

$$\langle \tau_{Lx} \tau_{Ly} \rangle_c = -\frac{x(1-y)}{L}(\rho_a - \rho_b)^2 \tag{18}$$

and shows that, as soon as the system is out of equilibrium, there are long range correlations.

5 The Large Deviation Function $\mathscr{F}(\rho(x))$ for the SSEP

For the SSEP (in one dimension), the functional $\mathscr{F}(\rho(x))$ is given by the following exact expression:

- At equilibrium, i.e. for $\rho_a = \rho_b = r$

$$\mathscr{F}(\rho(x)) = \int_0^1 B(\rho(x), r)dx \tag{19}$$

where

$$B(\rho, r) = (1-\rho)\log\frac{1-\rho}{1-r} + \rho\log\frac{\rho}{r}. \tag{20}$$

This can be derived easily. When $\rho_a = \rho_b = r$, the steady state is a Bernoulli measure where all the sites are occupied independently with probability r. Therefore if one divides a chain of length L into L/l intervals of length l, one has

$$\mathrm{Pro}(\rho_1, \ldots \rho_n) = \prod_i^{L/l} \frac{l!}{[l\rho_i]![l(1-\rho_i)]!} r^{l\rho_i}(1-r)^{l(1-\rho_i)} \tag{21}$$

and using Stirling's formula one gets (19), (20).

- In the non-equilibrium case, i.e. for $\rho_a \neq \rho_b$, it was shown in [2, 13, 14, 36] that

$$\mathscr{F}(\rho(x)) = \int_0^1 dx \left[B(\rho(x), F(x)) + \log\frac{F'(x)}{\rho_b - \rho_a} \right] \tag{22}$$

where the function $F(x)$ is the monotone solution of the differential equation

$$\rho(x) = F + \frac{F(1-F)F''}{F'^2} \tag{23}$$

satisfying the boundary conditions $F(0) = \rho_a$ and $F(1) = \rho_b$.

This expression shows that $\mathscr{F}$ is a *non-local* functional of the density profile $\rho(x)$ as $F(x)$ depends (in a non-linear way) on the profile $\rho(y)$ at all points y. For example if the difference $\rho_a - \rho_b$ is small, one can expand $\mathscr{F}$ and obtain an expression where the non-local character of the functional is clearly visible

$$\mathscr{F} = \int_0^1 dx\, B(\rho(x), \overline{\rho}(x)) + \frac{(\rho_a - \rho_b)^2}{[\rho_a(1-\rho_a)]^2} \int_0^1 dx \int_x^1 dy\, x(1-y)\big(\rho(x) - \overline{\rho}(x)\big)\big(\rho(y) - \overline{\rho}(y)\big) + O(\rho_a - \rho_b)^3 \tag{24}$$

where $\overline{\rho}(x)$ is the most likely profile given by

$$\overline{\rho}(x) = (1-x)\rho_a + x\rho_b. \tag{25}$$

A derivation of (22), (23) is described in Sects. 6, 7, 8.

6 The Matrix Ansatz for the Symmetric Exclusion Process

The matrix ansatz gives an algebraic way of calculating the exact weights [11, 33] of all the configurations in the steady state. In [12] it was shown that the probability of a microscopic configuration $\{\tau_1, \tau_2, \ldots, \tau_L\}$ can be written as the matrix element of a product of L matrices

$$\text{Pro}(\{\tau_1, \tau_2, \ldots \tau_L\}) = \frac{\langle W|X_1 X_2 \ldots X_L|V\rangle}{\langle W|(D+E)^L|V\rangle} \tag{26}$$

where the matrix X_i depends on the occupation τ_i of site i

$$X_i = \tau_i D + (1-\tau_i)E \tag{27}$$

and the matrices D and E satisfy the following algebraic rules

$$\begin{aligned} &DE - ED = D + E \\ &\langle W|(\alpha E - \gamma D) = \langle W| \\ &(\beta D - \delta E)|V\rangle = |V\rangle. \end{aligned} \tag{28}$$

Let us check on the simple example of Fig. 5 that expression (26) does give the steady state weights: if one chooses the configuration where the first p sites on the left are occupied and the remaining $L - p$ sites on the right are empty, the weight of this configuration is given by

$$\frac{\langle W|D^p E^{L-p}|V\rangle}{\langle W|(D+E)^L|V\rangle}. \tag{29}$$

For (26) to be the weights of all configurations in the steady state, one needs that the rate at which the system enters each configuration and the rate at which the system leaves it should be equal. In the case of the configuration whose weight is (29), this means that the following steady state identity should be satisfied (see Fig. 5):

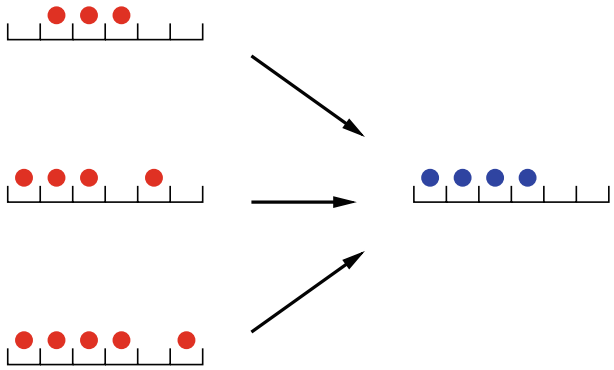

Fig. 5 The three configurations which appear on the left-hand side of (30) and from which one can jump to the configuration which appears on the right-hand side of (30)

$$\alpha \frac{\langle W|ED^{p-1}E^{L-p}|V\rangle}{\langle W|(D+E)^L|V\rangle} + \frac{\langle W|D^{p-1}EDE^{L-p-1}|V\rangle}{\langle W|(D+E)^L|V\rangle} + \beta \frac{\langle W|D^pE^{L-p-1}D|V\rangle}{\langle W|(D+E)^L|V\rangle}$$
$$= (\gamma + 1 + \delta) \frac{\langle W|D^pE^{L-p}|V\rangle}{\langle W|(D+E)^L|V\rangle}. \tag{30}$$

This equality is easy to check by rewriting (30) as

$$\frac{\langle W|(\alpha E - \gamma D)D^{p-1}E^{L-p}|V\rangle}{\langle W|(D+E)^L|V\rangle} - \frac{\langle W|D^{p-1}(DE - ED)E^{L-p-1}|V\rangle}{\langle W|(D+E)^L|V\rangle}$$
$$+ \frac{\langle W|D^pE^{L-p-1}(\beta D - \delta E)|V\rangle}{\langle W|(D+E)^L|V\rangle} = 0 \tag{31}$$

and by using (28). A similar reasoning [12] allows one to prove that the corresponding steady state identity holds for all the other configurations.

A priori one should construct the matrices D and E (which might be infinite-dimensional [12]) and the vectors $\langle W|$ and $|V\rangle$ satisfying (28) to calculate the weights (26) of the microscopic configurations. However these weights do not depend on the particular representation chosen and can be calculated directly from (28). This can be easily seen by using the two matrices A and B defined by

$$\begin{aligned} A &= \beta D - \delta E \\ B &= \alpha E - \gamma D \end{aligned} \tag{32}$$

which satisfy

$$AB - BA = (\alpha\beta - \gamma\delta)(D + E) = (\alpha + \delta)A + (\beta + \gamma)B. \tag{33}$$

For generic $\alpha, \beta, \gamma, \delta$, each product of D's and E's can be written as a sum of products of A's and B's which can be ordered using (33) by pushing all the A's to the right and all the B's to the left. One then gets a sum of terms of the form B^pA^q,

the matrix elements of which can be evaluated easily ($\langle W|B^p A^q|V\rangle = \langle W|V\rangle$) from (28) and (32).

With the weights (26) one can calculate the average density profile

$$\langle \tau_i \rangle = \frac{\langle W|(D+E)^{i-1} D (D+E)^{L-i}|V\rangle}{\langle W|(D+E)^L|V\rangle}$$

as well as all the correlation functions

$$\langle \tau_i \tau_j \rangle = \frac{\langle W|(D+E)^{i-1} D (D+E)^{j-i-1} D (D+E)^{L-j}|V\rangle}{\langle W|(D+E)^L|V\rangle}$$

and one can recover that way (15) and (17).

Using the fact that the average current between sites i and $i+1$ is given by

$$\langle J \rangle = \frac{\langle W|(D+E)^{i-1}(DE-ED)(D+E)^{L-i-1}|V\rangle}{\langle W|(D+E)^L|V\rangle} = \frac{\langle W|(D+E)^{L-1}|V\rangle}{\langle W|(D+E)^L|V\rangle}$$

(of course in the steady state the current does not depend on i) and from the expression (16) one can calculate the normalization

$$\frac{\langle W|(D+E)^L|V\rangle}{\langle W|V\rangle} = \frac{1}{(\rho_a - \rho_b)^L} \frac{\Gamma(L + \frac{1}{\alpha+\gamma} + \frac{1}{\beta+\delta})}{\Gamma(\frac{1}{\alpha+\gamma} + \frac{1}{\beta+\delta})} \tag{34}$$

where $\Gamma(z)$ is the usual Gamma function which satisfies $\Gamma(z+1) = z\Gamma(z)$. (See (3.11) of [14] for an alternative derivation of this expression.)

Remark 1. When $\rho_a = \rho_b = r$, the two reservoirs are at the same density and the steady state becomes the equilibrium (Gibbs) state of the lattice gas at this density r. In this case, the weights of the configurations are those of a Bernoulli measure at density r, that is

$$\text{Pro}(\{\tau_1, \tau_2, \ldots \tau_L\}) = \prod_{i=1}^{L} [r\tau_i + (1-r)(1-\tau_i)]. \tag{35}$$

This case is a limit where the matrices D and E commute (it can be recovered by making all the calculations with the matrices (26), (28) for $\rho_a \neq \rho_b$ and by taking the limit $\rho_a \to \rho_b$ in the final expressions, as all the expectations, for a lattice of finite size L, are rational functions of ρ_a and ρ_b).

Remark 2. Here the discussion is limited to the symmetric exclusion process and other diffusive systems. The matrix approach can however be extended to the asymmetric exclusion process [12] and the methods of Sects. 7 and 8 generalized to obtain the large deviation function of the density in presence of an asymmetry [15, 16, 20].

7 Additivity as a Consequence of the Matrix Ansatz

In this section we are going to establish, starting from the matrix ansatz (26), (28), an identity (42) which will relate (in Sect. 8) the large deviation function $\mathscr{F}$ of a system to those of its subsystems.

As in (26) the weight of every configuration is written as the matrix element of a product of L matrices, one can try to insert at a position L' a complete basis in order to relate the properties of a lattice of L sites to those of two subsystems of sizes L' and $L - L'$. To do so let us introduce the following left and right eigenvectors of the operators $\rho_a E - (1 - \rho_a)D$ and $(1 - \rho_b)D - \rho_b E$

$$\begin{aligned} \langle \rho_a, a|[\rho_a E - (1 - \rho_a)D] &= a\langle \rho_a, a| \\ [(1 - \rho_b)D - \rho_b E]|\rho_b, b\rangle &= b|\rho_b, b\rangle. \end{aligned} \tag{36}$$

It is easy to see, using (13) and (28), that the vectors $\langle W|$ and $|V\rangle$ are given by

$$\begin{aligned} \langle W| &= \langle \rho_a, (\alpha + \gamma)^{-1}| \\ |V\rangle &= |\rho_b, (\beta + \delta)^{-1}\rangle. \end{aligned} \tag{37}$$

It is then possible to show, using simply the fact (28) that $DE - ED = D + E$ and the definition of the eigenvectors (36), that (for $\rho_b < \rho_a$)

$$\begin{aligned} &\frac{\langle \rho_a, a|Y_1 Y_2|\rho_b, b\rangle}{\langle \rho_a, a|\rho_b, b\rangle} \\ &= \oint_{\rho_b<|\rho|<\rho_a} \frac{d\rho}{2i\pi} \frac{(\rho_a - \rho_b)^{a+b}}{(\rho_a - \rho)^{a+b}(\rho - \rho_b)} \frac{\langle \rho_a, a|Y_1|\rho, b\rangle}{\langle \rho_a, a|\rho, b\rangle} \frac{\langle \rho, 1 - b|Y_2|\rho_b, b\rangle}{\langle \rho, 1 - b|\rho_b, b\rangle} \end{aligned} \tag{38}$$

where Y_1 and Y_2 are arbitrary polynomials of the matrices D and E.

To prove (38) it is sufficient to choose Y_1 of the form $[\rho_a E - (1-\rho_a)D]^n [D+E]^{n'}$ (clearly any polynomial of the matrices D and E can be rewritten as a polynomial of $A \equiv D + E$ and $B \equiv \rho_a E - (1 - \rho_a)D$. Then as $AB - BA = A$, which is a consequence of $DE - ED = D + E$, one can push all the A's to the right and all the B's to the left. Therefore any polynomial can be written as a sum of terms of the form $[\rho_a E - (1 - \rho_a)D]^n [D + E]^{n'}$). Similarly one can choose Y_2 of the form $[D + E]^{n''}[(1 - \rho_b)D - \rho_b E]^{n'''}$. Then proving (38) for such choices of Y_1 and Y_2 reduces to proving

$$\begin{aligned} &\frac{\langle \rho_a, a|(D + E)^{n'+n''}|\rho_b, b\rangle}{\langle \rho_a, a|\rho_b, b\rangle} \\ &= \oint_{\rho_b<|\rho|<\rho_a} \frac{d\rho}{2i\pi} \frac{(\rho_a - \rho_b)^{a+b}}{(\rho_a - \rho)^{a+b}(\rho - \rho_b)} \frac{\langle \rho_a, a|(D + E)^{n'}|\rho, b\rangle}{\langle \rho_a, a|\rho, b\rangle} \\ &\quad \times \frac{\langle \rho, 1 - b|(D + E)^{n''}|\rho_b, b\rangle}{\langle \rho, 1 - b|\rho_b, b\rangle}. \end{aligned} \tag{39}$$

From (34) one has

$$\frac{\langle \rho_a, a|(D+E)^L|\rho, b\rangle}{\langle \rho_a, a|\rho, b\rangle} = \frac{\Gamma(L+a+b)}{(\rho_a-\rho_b)^L \Gamma(a+b)}. \tag{40}$$

Then (38) and (39) follow as one can easily check that

$$\frac{\Gamma(n'+n''+a+b)}{(\rho_a-\rho_b)^{n'+n''}} = \oint_{\rho_b<|\rho|<\rho_a} \frac{d\rho}{2i\pi} \frac{(\rho_a-\rho_b)^{a+b}}{(\rho_a-\rho)^{a+b+n'}(\rho-\rho_b)^{n''+1}} \frac{\Gamma(n'+a+b)\Gamma(n''+1)}{\Gamma(a+b)}. \tag{41}$$

If one normalizes (38) by (34) one gets

$$\frac{\langle \rho_a, a|Y_1 Y_2|\rho_b, b\rangle}{\langle \rho_a, a|(D+E)^{L+L'}|\rho_b, b\rangle} = \frac{\Gamma(L+a+b)\Gamma(L'+1)}{\Gamma(L+L'+a+b)} \oint_{\rho_b<|\rho|<\rho_a} \frac{d\rho}{2i\pi} \frac{(\rho_a-\rho_b)^{a+b+L+L'}}{(\rho_a-\rho)^{a+b+L}(\rho-\rho_b)^{1+L'}} \times \frac{\langle \rho_a, a|Y_1|\rho, b\rangle}{\langle \rho_a, a|(D+E)^L|\rho, b\rangle} \frac{\langle \rho, 1-b|Y_2|\rho_b, b\rangle}{\langle \rho, 1-b|(D+E)^{L'}|\rho_b, b\rangle}. \tag{42}$$

This gives an exact relation between the steady state properties of a system of size $L+L'$ and those of its subsystems.

8 Large Deviation Function of Density Profiles

We are now going to see how the expression (22), (23) of the large deviation functional $\mathscr{F}(\rho(x))$ can be obtained for the SSEP from the additivity relation (42).

One can divide a chain of L sites into n boxes of linear size l (there are of course $n = L/l$ such boxes) and try to determine the probability of finding a certain density profile $\{\rho_1, \rho_2, \ldots, \rho_n\}$, i.e. the probability of seeing $l\rho_1$ particles in the first box, $l\rho_2$ particles in the second box, $\ldots l\rho_n$ in the nth box. For large L one expects (see (7)) the following L dependence of this probability

$$\mathrm{Pro}_L(\rho_1, \ldots, \rho_n|\rho_a, \rho_b) \sim \exp[-L\mathscr{F}_n(\rho_1, \rho_2, \ldots, \rho_n|\rho_a, \rho_b)]. \tag{43}$$

If one defines a reduced coordinate x by

$$i = Lx \tag{44}$$

and if one takes the limit $l \to \infty$ with $l \ll L$ so that the number of boxes becomes infinite, one gets as in (9) the large deviation functional $\mathscr{F}(\rho(x))$

$$\mathrm{Pro}_L(\{\rho(x)\}) \sim \exp[-L\mathscr{F}(\{\rho(x)\}|\rho_a, \rho_b)]. \tag{45}$$

To derive (22), (23) (for simplicity we do it here in the particular case where $a + b = 1$, i.e. $\frac{1}{\alpha+\gamma} + \frac{1}{\beta+\delta} = 1$, and $\rho_b < \rho_a$ but the extension to other cases is easy) one can use (42) when Y_1 represents a sum over all configurations of the first kl sites with a density ρ_1 in the first l sites, $\dots \rho_k$ in the k-th l sites, and Y_2 a similar sum for the $(n-k)l$ remaining sites.

$$\begin{aligned} &P_{nl}(\rho_1, \rho_2, \dots, \rho_n|\rho_a, \rho_b) \\ &\quad = \frac{(kl)!((n-k)l)!}{(nl)!} \oint_{\rho_b<|\rho|<\rho_a} \frac{d\rho}{2i\pi} \\ &\qquad \times \frac{(\rho_a - \rho_b)^{nl+1}}{(\rho_a - \rho)^{kl+1}(\rho - \rho_b)^{(n-k)l+1}} P_{kl}(\rho_1 \dots \rho_k|\rho_a, \rho) \\ &\qquad \times P_{(n-k)l}(\rho_{k+1} \dots \rho_n|\rho, \rho_b). \end{aligned} \tag{46}$$

Note that in (46) the density ρ has become a complex variable. This is not a difficulty as all the weights (and therefore the probabilities which appear in (46)) are rational functions of ρ_a and ρ_b.

For large nl, if one writes $k = nx$, one gets by evaluating (46) at the saddle point

$$\begin{aligned} &\mathscr{F}_n(\rho_1, \rho_2, \dots, \rho_n|\rho_a, \rho_b) \\ &\quad = \max_{\rho_b<F<\rho_a} x\mathscr{F}_k(\rho_1, \dots, \rho_k|\rho_a, F) + (1-x)\mathscr{F}_{n-k}(\rho_{k+1}, \dots, \rho_n|F, \rho_b) \\ &\qquad + x\log\left(\frac{\rho_a - F}{x}\right) + (1-x)\log\left(\frac{F - \rho_b}{1-x}\right) - \log(\rho_a - \rho_b). \end{aligned} \tag{47}$$

(To estimate (46) by a saddle point method, one should find the value F of ρ which *maximizes* the integrand over the contour. As the contour is perpendicular to the real axis at their crossing point, this becomes *a minimum* when ρ varies along the real axis.) If one repeats the same procedure n times, one gets

$$\begin{aligned} &\mathscr{F}_n(\rho_1, \rho_2, \dots, \rho_n|\rho_a, \rho_b) \\ &\quad = \max_{\rho_b=F_0<F_1<\dots<F_i<\dots<F_n=\rho_a} \frac{1}{n}\sum_{i=1}^{n} \mathscr{F}_1(\rho_i|F_{i-1}, F_i) \\ &\qquad + \log\left(\frac{(F_{i-1} - F_i)n}{\rho_a - \rho_b}\right). \end{aligned} \tag{48}$$

For large n, as F_i is monotone, the difference $F_{i-1} - F_i$ is small for almost all i and one can replace $\mathscr{F}_1(\rho_i|F_{i-1}, F_i)$ by its equilibrium value $\mathscr{F}_1(\rho_i|F_i, F_i) = B(\rho_i, F_i)$. If one write F_i as a function of i/n

$$F_i = F\left(\frac{i}{n}\right) \tag{49}$$

(48) becomes

$$\mathscr{F}(\{\rho(x)\}|\rho_a,\rho_b) = \max_{F(x)} \int_0^1 dx \left[B(\rho(x), F(x)) + \log \frac{F'(x)}{\rho_b - \rho_a} \right] \tag{50}$$

where the maximum is over all the monotone functions $F(x)$ which satisfy $F(0) = \rho_a$ and $F(1) = \rho_b$ and one gets (22), (23).

Other derivations of (50) are given in [2, 13, 14, 36].

9 Non-locality of the Large Deviation Functional of the Density and Long Range Correlations

A feature characteristic of non-equilibrium systems is the presence of weak long range correlations [19, 34]. For example for the SSEP, we saw in (17) that for large L the correlation function of the density is given for $0 < x < y < 1$

$$\langle \rho(x)\rho(y)\rangle_c = -\frac{(\rho_a - \rho_b)^2}{L} x(1-y). \tag{51}$$

We are now going to see that the presence of these long range correlations is directly related to the non-locality of the large deviation functional $\mathscr{F}$. Let us introduce the generating function $\mathscr{G}(\{\alpha(x)\})$ of the density defined by

$$\exp\left[L\mathscr{G}(\{\alpha(x)\})\right] = \left\langle \exp\left[L \int_0^1 \alpha(x)\rho(x)dx \right] \right\rangle \tag{52}$$

where $\alpha(x)$ is an arbitrary function and $\langle . \rangle$ denotes an average over the profile $\rho(x)$ in the steady state. As the probability of this profile has the form (45), the average in (52) is dominated, for large L, by an optimal profile which depends on $\alpha(x)$ and $\mathscr{G}$ is the Legendre transform of $\mathscr{F}$

$$\mathscr{G}(\{\alpha(x)\}) = \max_{\{\rho(x)\}} \left[\int_0^1 \alpha(x)\rho(x)dx - \mathscr{F}(\{\rho(x)\}) \right]. \tag{53}$$

It is clear from (53) that if the large deviation $\mathscr{F}$ is local (as in (12)), then the generating function $\mathscr{G}$ is also local.

By taking derivatives of (52) with respect to $\alpha(x)$ one gets that the average profile and the correlation functions are given by

$$\overline{\rho}(x) \equiv \langle \rho(x)\rangle = \left.\frac{\delta \mathscr{G}}{\delta \alpha(x)}\right|_{\alpha(x)=0} \tag{54}$$

$$\langle \rho(x)\rho(y)\rangle_c \equiv \langle \rho(x)\rho(y)\rangle - \langle \rho(x)\rangle\langle \rho(y)\rangle = \frac{1}{L} \left.\frac{\delta^2 \mathscr{G}}{\delta\alpha(x)\delta\alpha(y)}\right|_{\alpha(x)=0}. \tag{55}$$

This shows that the non-locality of $\mathscr{G}$ and therefore the non-locality of $\mathscr{F}$ is directly related to the existence of long range correlations.

To understand the L dependence in (55) let us assume that the non-local functional $\mathscr{G}$ can be expanded as

$$\mathscr{G}(\alpha(x)) = \int_0^1 dx A(x)\alpha(x) + \int_0^1 dx B(x)\alpha(x)^2 + \int_0^1 dx \int_x^1 dy C(x, y)\alpha(x)\alpha(y) + \cdots . \tag{56}$$

If one comes back to a lattice gas of L sites with a number n_i of particles on site i and one considers the generating function of these occupation numbers, one has for large L

$$\log\left[\left\langle \exp \sum_i \alpha_i n_i \right\rangle\right] \simeq L\mathscr{G}(\alpha(x)) \tag{57}$$

when α_i is a slowly varying function of i of the form $\alpha_i = \alpha(i/L)$. By expanding the l.h.s. of (57) in powers of the α_i one has

$$\log\left[\left\langle \exp \sum_i \alpha_i n_i \right\rangle\right] = \sum_{i=1}^{L} A_i\alpha_i + \sum_{i=1}^{L} B_i\alpha_i^2 + \sum_{i<j} C_{i,j}\alpha_i\alpha_j + \cdots \tag{58}$$

and therefore

$$\langle n_i \rangle = A_i; \qquad \langle n_i^2 \rangle_c = 2B_i; \qquad \langle n_i n_j \rangle_c = C_{i,j}. \tag{59}$$

Comparing (56) and (58) in (57) one can see that

$$C_{i,j} = \frac{1}{L} C\left(\frac{i}{L}, \frac{j}{L}\right) \tag{60}$$

which leads to (55).

A similar reasoning would show that

$$\langle \rho(x_1)\rho(x_2)\ldots\rho(x_k)\rangle_c = \frac{1}{L^{k-1}} \left.\frac{\delta^k \mathscr{G}}{\delta\alpha(x_1)\ldots\delta\alpha(x_k)}\right|_{\alpha(x)=0}. \tag{61}$$

This $1/L^{k-1}$ dependence of the k point function can indeed be proved in the SSEP [19]. We see that all the correlation functions can in principle be obtained by expanding, when this expansion is meaningful (see [15, 16] for counter-examples), the large deviation function $\mathscr{G}$ in powers of $\alpha(x)$.

10 The Macroscopic Fluctuation Theory

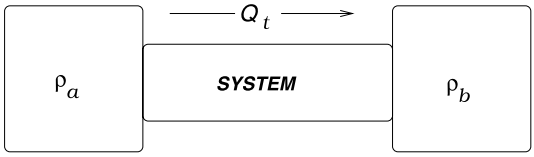

Fig. 6 System in contact with two reservoirs of particles at densities ρ_a and ρ_b

For a general diffusive one dimensional system (Fig. 6) of linear size L the average current and the fluctuations of this current near equilibrium can be characterized by two quantities $D(\rho)$ and $\sigma(\rho)$ defined by

$$\lim_{t\to\infty} \frac{\langle Q_t \rangle}{t} = \frac{D(\rho)}{L}(\rho_a - \rho_b) \quad \text{for } (\rho_a - \rho_b) \text{ small} \tag{62}$$

$$\lim_{t\to\infty} \frac{\langle Q_t^2 \rangle}{t} = \frac{\sigma(\rho)}{L} \quad \text{for } \rho_a = \rho_b \tag{63}$$

where Q_t is the total number of particles transferred from the left reservoir to the system during time t.

Bertini, De Sole, Gabrielli, Jona-Lasinio and Landim [1–3] have developed a general approach, *the macroscopic fluctuation theory*, to calculate the large deviation functional $\mathscr{F}$ of the density (9) in the non-equilibrium steady state of a system in contact with two (or more) reservoirs as in Fig. 6. Their approach can be briefly sketched as follows. For diffusive systems (such as the SSEP), the density $\rho_i(t)$ near position i at time t and the total flux $Q_i(t)$ flowing through position i between time 0 and time t are, for a large system of size L and for times of order L^2, scaling functions of the form

$$\rho_i(t) = \widehat{\rho}\left(\frac{i}{L}, \frac{t}{L^2}\right), \quad \text{and} \quad Q_i(t) = L\,\widehat{Q}\left(\frac{i}{L}, \frac{t}{L^2}\right). \tag{64}$$

(Note that due to the conservation of the number of particles, the scaling form of $\rho_i(t)$ implies the scaling form of $Q_i(t)$.) If one introduces the instantaneous (rescaled) current defined by

$$\widehat{j}(x,\tau) = \frac{\partial \widehat{Q}(x,\tau)}{\partial \tau} \tag{65}$$

the conservation of the number of particles implies that

$$\frac{\partial \widehat{\rho}(x,\tau)}{\partial \tau} = -\frac{\partial^2 \widehat{Q}(x,\tau)}{\partial \tau\, \partial x} = -\frac{\partial \widehat{j}(x,\tau)}{\partial x}. \tag{66}$$

As the starting point [28] of the Bertini, De Sole, Gabrielli, Jona-Lasinio and Landim [1–3] approach, one can write the probability of observing a density profile $\widehat{\rho}(x,s)$ and a current $\widehat{j}(x,s)$ (related by (66)) over a time interval (t_1,t_2) is given by

$$\mathrm{Pro}(\widehat{\rho}(x,s),\widehat{j}(x,s)) \sim \exp\left\{-L\int_{t_1/L^2}^{t_2/L^2} ds\int_0^1 dx\frac{[\widehat{j}+D(\widehat{\rho})\frac{d\widehat{\rho}}{dx}]^2}{2\sigma(\widehat{\rho})}\right\}. \tag{67}$$

They showed that to observe a certain deviation $\rho(x)$ of the density profile at time $t=L^2\tau$, one has to find out how this fluctuation is produced. For large L, there is an optimal path $\widehat{\rho}(x,s)$ for $-\infty<s<\tau$ in the space of profiles which goes from the most likely steady state profile $\overline{\rho}(x)$ to the desired profile $\rho(x)$. In other words

$$\mathrm{Pro}(\rho(x)) \sim \max_{\widehat{\rho}(x,s)} \exp\left\{-L\int_{-\infty}^{t} ds\int_0^1 dx\frac{[\widehat{j}+D(\widehat{\rho})\frac{d\widehat{\rho}}{dx}]^2}{2\sigma(\widehat{\rho})}\right\} \tag{68}$$

where the current $\widehat{j}(x,s)$ is related to the density profile $\widehat{\rho}(x,s)$ by (66) and the optimal path $\widehat{\rho}(x,s)$ satisfies

$$\widehat{\rho}(x,-\infty)=\overline{\rho}(x) \tag{69}$$

$$\rho(x,t)=\rho(x). \tag{70}$$

Comparing (68) with (45) this gives

$$\mathscr{F}(\rho(x)) = \min_{\widehat{\rho}(x,s)}\int_{-\infty}^{\tau} ds\int_0^1 dx\frac{[\widehat{j}+D(\widehat{\rho})\frac{d\widehat{\rho}}{dx}]^2}{2\sigma(\widehat{\rho})} \tag{71}$$

Finding this optimal path $\widehat{\rho}(x,s)$, $\widehat{j}(x,s)$ is usually a hard problem and so far one does not know how to find an expression more explicit than (71) of the functional $\mathscr{F}$ for general $D(\rho)$ and $\sigma(\rho)$. Bertini et al. [1] were however able to show that for the SSEP this approach allows one to recover the expressions (22), (23).

Apart for the SSEP, the large deviation functional $\mathscr{F}$ of the density is so far known only in very few cases: the Kipnis Marchioro Presutti model [5, 27] the weakly asymmetric exclusion process [20] and the ABC model [10, 24] on a ring for equal densities of the three species.

11 Large Deviation of the Current

As we did it in (3) for the density, one can define the large deviation function of the current of particles for a system in contact with two reservoirs at densities ρ_a and ρ_b as in Fig. 6 (or of the heat current for a system in contact with two heat baths as in Fig. 1). The probability of observing during a long time t an average current j takes the form

$$\text{Pro}\left(\frac{Q_t}{t} = j\right) \sim e^{-tF(j)} \tag{72}$$

where $F(j)$ is the large deviation function of the current j. This large deviation function $F(j)$ has a shape similar to $a(\rho)$ in Fig. 2, with a minimum at some value $\langle J\rangle$, the typical value of the current, where $F(\langle J\rangle) = 0$. The knowledge of $F(j)$ determines, by expanding around $\langle J\rangle$, all the cumulants of Q_t for large t.

In the non-equilibrium steady state of systems such as those of Figs. 1 and 6, the large deviation function $F(j)$ satisfies *the fluctuation theorem* [22, 23, 25, 30, 31]. For diffusive systems characterized by the two functions $D(\rho)$ and $\sigma(\rho)$ as in (62) and (63), this tells us that $F(j)$ satisfies

$$F(j) - F(-j) = j\int_{\rho_b}^{\rho_a} \frac{D(\rho)}{\sigma(\rho)} d\rho. \tag{73}$$

Therefore even if $F(j)$ is a complicated function, the difference $F(j)-F(-j)$ is, as predicted by the fluctuation theorem, linear in j, with a universal coefficient which depends only on ρ_a and ρ_b.

12 Generalized Detailed Balance and the Fluctuation Theorem

For systems such as the SSEP (see Sect. 4) with stochastic dynamics given by a Markov process the evolution is specified by a transition matrix $W(C', C)$ which represents the rate at which the system jumps from a configuration C to a configuration C' (i.e. the probability that the system jumps from C to C' during an infinitesimal time interval dt is $W(C', C)dt$). The probability $P_t(C)$ of finding the system in configuration C at time t evolves therefore according to the Master equation

$$\frac{dP_t(C)}{dt} = \sum_{C'} W(C, C')P_t(C') - W(C', C)P_t(C). \tag{74}$$

One can then wonder what should be assumed on the transition matrix $W(C', C)$ to describe a system in contact with one or several heat baths (as in Fig. 1).

At equilibrium, (i.e. when the system is in contact with a single heat bath at temperature T) one usually requires that the transition matrix satisfies *detailed balance*

$$W(C', C)e^{-\frac{E(C)}{kT}} = W(C, C')e^{-\frac{E(C')}{kT}}. \tag{75}$$

This ensures the time reversal symmetry of the microscopic dynamics: at equilibrium (i.e. if the initial condition is chosen according to (1)), the probability of observing any given history of the system $\{C_s, 0 < s < t\}$ is equal to the probability of observing the reversed history

$$\text{Pro}(\{C_s, 0 < s < t\}) = \text{Pro}(\{C_{t-s}, 0 < s < t\}). \tag{76}$$

Therefore if ϵ is the energy transferred from the heat bath at temperature T to the system, and $W_\epsilon(C', C)$ is the rate at which the system jumps during dt from C to C' by receiving an energy ϵ from the heat bath, one can rewrite the detailed balance condition (75) as

$$W_\epsilon(C', C) = e^{-\frac{\epsilon}{kT}} W_{-\epsilon}(C, C'). \tag{77}$$

If detailed balance gives a good description of the coupling with a single heat bath at temperature T, the straightforward generalization of (77) for a system coupled to two heat baths at unequal temperatures like in Fig. 1 is [8]

$$W_{\epsilon_a,\epsilon_b}(C', C) = e^{-\frac{\epsilon_a}{kT_a}-\frac{\epsilon_b}{kT_b}} W_{-\epsilon_a,-\epsilon_b}(C, C') \tag{78}$$

where ϵ_a, ϵ_b are the energies transferred from the heat baths at temperatures T_a, T_b to the system when the system jumps from configuration C to configuration C'. By comparing with (77), this simply means that the exchanges of energy with the heat bath at temperature T_a tend to equilibrate the system at temperature T_a and the exchanges with the heat bath at temperature T_b tend to equilibrate the system at temperature T_b.

For a system in contact with two reservoirs of particles at fugacities $z(\rho_a)$ and $z(\rho_b)$, as in Fig. 1, *the generalized detailed balance* (78) becomes

$$W_{q_a,q_b}(C', C) = z(\rho_a)^{q_a} z(\rho_b)^{q_b} W_{-q_a,-q_b}(C, C') \tag{79}$$

where q_a and q_b are the numbers of particles transferred from the two reservoirs to the system when the system jumps from configuration C to configuration C'. It is easy [8] to show that the fluctuation theorem

$$F(j) - F(-j) = j(\log z(\rho_a) - \log z(\rho_b)) \tag{80}$$

is, for Markov processes, a simple consequence of the generalized detailed balance (79). For diffusive systems comparing (73) and (80) implies that

$$\frac{d \log z(\rho)}{d\rho} = 2\frac{D(\rho)}{\sigma(\rho)}$$

which shows [8] that the ratio $D(\rho)/\sigma(\rho)$ is related (see [8, 35]) to the equilibrium compressibility at density ρ.

From the definition of the dynamics of the SSEP, it is easy to check that it satisfies (79) with

$$z(\rho_a) = \frac{\alpha}{\gamma}; \qquad z(\rho_b) = \frac{\delta}{\beta} \tag{81}$$

13 Current Fluctuations in the SSEP

In the long time limit the generating function of the total charge Q_t transferred from the left reservoir to the system during time t grows exponentially with time

$$\left\langle e^{\lambda Q_t} \right\rangle \sim e^{\mu(\lambda) t} \tag{82}$$

where $\mu(\lambda)$ is related to the large deviation function $F(j)$ by a Legendre transformation

$$\mu(\lambda) = \max_j [\lambda j - F(j)]. \tag{83}$$

Because the evolution is Markovian, $\mu(\lambda)$ can be determined as the largest eigenvalue of a certain matrix [17]: among the matrix elements $W(\mathscr{C}, \mathscr{C}')$ which appear in (74), some correspond to exchanges of particles with the left reservoir and some represent internal moves in the bulk or exchanges with the right reservoir. One can decompose the matrix $W(\mathscr{C}, \mathscr{C}')$ into three matrices

$$W(\mathscr{C}, \mathscr{C}') = W_1(\mathscr{C}, \mathscr{C}') + W_0(\mathscr{C}, \mathscr{C}') + W_{-1}(\mathscr{C}, \mathscr{C}') \tag{84}$$

where the index is the number of particles transferred from the left reservoir to the system during time dt, when the system jumps from the configuration $\mathscr{C}'$ to the configuration $\mathscr{C}$. One can then show [17] that $\mu(\lambda)$ is simply the largest eigenvalue of the matrix

$$e^{\lambda} W_1 + W_0 + e^{-\lambda} W_{-1}. \tag{85}$$

The steady state weights $P(\mathscr{C})$ for the SSEP are known exactly [12–14]: they determine the eigenvector of the matrix $e^{\lambda} W_1 + W_0 + e^{-\lambda} W_{-1}$ associated to the eigenvalue $\mu(\lambda)$ when $\lambda = 0$.

In [17] a perturbation theory was developed to calculate $\mu(\lambda)$ in powers of λ. The main outcome of this perturbation theory is that $\mu(\lambda)$, which in principle depends on L, λ and on the four parameters α, β, γ, δ, takes for large L a simple form

$$\mu(\lambda) = \frac{1}{L} R(\omega) + O\left(\frac{1}{L^2}\right) \tag{86}$$

where ω is defined by

$$\omega = (e^{\lambda} - 1)\rho_a + (e^{-\lambda} - 1)\rho_b - (e^{\lambda} - 1)(1 - e^{-\lambda})\rho_a \rho_b. \tag{87}$$

The perturbation theory gives up to fourth order in ω

$$R(\omega) = \omega - \frac{\omega^2}{3} + \frac{8\omega^3}{45} - \frac{4\omega^4}{35} + O(\omega^5). \tag{88}$$

The fact that $\mu(\lambda)$ depends only on ρ_a, ρ_b and λ through the single parameter ω is the outcome of the calculation, but so far there is no physical explanation why it is so.

From the knowledge of $R(\omega)$ up to fourth order in ω, one can determine the first four cumulants of the integrated current Q_t for arbitrary ρ_a and ρ_b:

For $\rho_a = \rho_b = \frac{1}{2}$ which corresponds to an equilibrium case with the same density $1/2$ in the two reservoirs, all odd cumulants vanish as they should and one finds from (86), (87), (88) that

$$\frac{\langle Q_t^2 \rangle_c}{t} = \frac{1}{2L} + O\left(\frac{1}{L^2}\right) \tag{89}$$

$$\frac{\langle Q_t^4 \rangle_c}{t} = O\left(\frac{1}{L^2}\right). \tag{90}$$

Because $\mu(\lambda)$ depends on the parameters ρ_a, ρ_b and λ through the single parameter ω, if one knows $\mu(\lambda)$ for one single choice of ρ_a and ρ_b, then (86)–(88) determine $\mu(\lambda)$ for all other choices of ρ_a, ρ_b.

In [17], it was *conjectured* that for the particular case $\rho_a = \rho_b = \frac{1}{2}$, not only the fourth cumulant vanishes as in (90), but also all the higher cumulants vanish, so that the distribution of Q_t is Gaussian (to leading order in $1/L$). This conjecture fully determines the function $R(\omega)$ to be

$$R(\omega) = \left[\log\left(\sqrt{1+\omega} + \sqrt{\omega}\right)\right]^2. \tag{91}$$

14 The Additivity Principle

One can formulate another conjecture, the additivity principle [6], based on a simple physical picture, which leads to the same expression (86), (87), (91) as predicted by the previous conjecture and can be generalized to other diffusive systems.

For a system of length $L + L'$ in contact with two reservoirs of particles at densities ρ_a and ρ_b, the probability of observing, during a long time t, an integrated current $Q_t = jt$ has the following form (72)

$$\mathrm{Pro}_{L+L'}(j, \rho_a, \rho_b) \sim e^{-t F_{L+L'}(j, \rho_a, \rho_b)}. \tag{92}$$

The idea of the additivity principle [6] is to try to relate the large deviation function $F_{L+L'}(j, \rho_a, \rho_b)$ of the current to the large deviation functions of subsystems by writing that for large t

$$\mathrm{Pro}_{L+L'}(j, \rho_a, \rho_b) \sim \max_{\rho} \left[\mathrm{Pro}_L(j, \rho_a, \rho) \times \mathrm{Pro}_{L'}(j, \rho, \rho_b)\right]. \tag{93}$$

This means that the probability of transporting a current j over a distance $L + L'$ between two reservoirs at densities ρ_a and ρ_b is the same (up to boundary effects which give for large L subleading contributions) as the probability of transporting the same current j over a distance L between two reservoirs at densities ρ_a and ρ times the probability of transporting the current j over a distance L' between

two reservoirs at densities ρ and ρ_b. One can then argue that choosing the optimal ρ makes this probability maximum. From (93) one gets the following additivity property of the large deviation function

$$F_{L+L'}(j, \rho_a, \rho_b) = \min_{\rho} \left[F_L(j, \rho_a, \rho) + F_{L'}(j, \rho, \rho_b) \right]. \tag{94}$$

If one accepts this additivity property (94) of the large deviation function, one can cut the system into more and more pieces so that [6] when these pieces have length Ldx, one gets

$$F_L(j, \rho_a, \rho_b) = \frac{1}{L} \min_{\rho(x)} \left[\int_0^1 F_{Ldx}(j, \rho(x), \rho(x+dx)) dx \right] \tag{95}$$

where the optimal $\rho(x)$ should satisfy $\rho(0) = \rho_a$ and $\rho(1) = \rho_b$.

Now for a small current (in fact the currents j for which one can use the additivity principle are of order $1/L$), and $\rho(x+dx) - \rho(x)$ small, one expects (62), (63) that for $Ldx \gg 1$ that

$$\begin{aligned} F_{Ldx}(j, \rho(x), \rho(x+dx)) &\simeq \frac{[j - D(\rho(x)) \frac{\rho(x) - \rho(x+dx)}{Ldx}]^2}{2 \frac{\sigma(\rho(x))}{Ldx}} \\ &\simeq \frac{dx}{L} \frac{(Lj + D(\rho(x))\rho'(x))^2}{2\sigma(\rho(x))} \end{aligned}$$

and therefore (95) becomes

$$F_L(j, \rho_a, \rho_b) = \frac{1}{L} \max_{\rho(x)} \left[\int_0^1 \frac{[Lj + D(\rho(x))\rho'(x)]^2}{2\sigma(\rho(x))} dx \right]. \tag{96}$$

Using the fact that for the SSEP $D(\rho) = 1$ and $\sigma(\rho) = 2\rho(1-\rho)$, one can recover [6] from (96) the above expression (86), (87), (91). For more general diffusive systems, one can also determine all the cumulants of the integrated current for arbitrary ρ_a and ρ_b. For example [6, 8]

$$\frac{\langle Q_t^4 \rangle_c}{t} = \frac{1}{L} \frac{3(5I_4 I_1^2 - 14 I_1 I_2 I_3 + 9 I_2^3)}{I_1^5} \tag{97}$$

where

$$I_n = \int_{\rho_b}^{\rho_a} D(\rho) \sigma(\rho)^{n-1} d\rho. \tag{98}$$

There are restrictions [4] on $\sigma(\rho)$ and $D(\rho)$ for (96) to be valid: in particular $F_L(j, \rho_a, \rho_b)$, defined in (92), is a convex function of j. For some $\sigma(\rho)$ and $D(\rho)$ one has to replace the expression (96) of $F_L(j, \rho_a, \rho_b)$ by its convex envelope. It has also been realized [4, 7, 8] that starting from the macroscopic fluctuation theory, the large deviation function of the current should be given by

$$F_L(j, \rho_a, \rho_b) = \frac{1}{L} \lim_{\tau \to \infty} \left[\min_{\widehat{\rho}(x,s), \widehat{j}(x,s)} \int_{-\infty}^{\tau} ds \int_0^1 dx \frac{[\widehat{j} + D(\widehat{\rho}) \frac{d\widehat{\rho}}{dx}]^2}{2\sigma(\widehat{\rho})} \right] \quad (99)$$

where the minimum is over all the time dependent density and current profiles $\widehat{\rho}$, $\widehat{j}$. Therefore the expression (96) is valid only when the optimal profiles in (99) are time independent. It does happen [7, 8] phase transitions beyond which these optimal profiles become time dependent and (96) is no longer valid.

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Robust Heterodimensional Cycles and Tame Dynamics

Lorenzo J. Díaz

Dedicated to Paul Schweitzer (now 70 years young)

Abstract A diffeomorphism f has a heterodimensional cycle if there are hyperbolic sets Λ and Σ with different indices (dimension of the unstable bundle) such that the unstable manifold of Λ meets the stable one of Σ and vice-versa. This cycle has co-index one if $\text{index}(\Lambda) = \text{index}(\Sigma) \pm 1$ and is robust if, for every g close to f, the continuations of Λ and Σ for g have a cycle. In the C^1-setting, we discuss the generation of robust heterodimensional cycles by heterodimensional ones and obtain some consequences of this phenomenon for tame dynamics.

1 Robust Heterodimensional Cycles

1.1 General Setting

In [37, 38], Smale conjectured that the structurally stable diffeomorphisms of a closed manifold are dense. He later disproved his conjecture in [39] by exhibiting a three-dimensional manifold and a C^1-open set of non-structurally stable diffeomorphisms. Smale's example was strengthened in [4], by constructing a C^1-open set $\mathscr{U}$ of diffeomorphisms defined on the product $\mathbb{T}^2 \times \mathbb{S}^2$ of a two torus and a two sphere having cycles. As a consequence, the diffeomorphisms in $\mathscr{U}$ do not verify Axiom A and thus Axiom A is not generic (Axiom A diffeomorphisms does not contain a residual subset $\text{Diff}^1(\mathbb{T}^2 \times \mathbb{S}^2)$).

Recall that, for C^1-generic diffeomorphisms, all periodic points are hyperbolic and they form a dense subset of the limit set (see [21, 32]). Axiom A demands that in addition the hyperbolic structures on the periodic points fit together nicely.

Lorenzo J. Díaz
Departamento de Matemática, PUC-Rio, Marquês de São Vicente 225, Gávea, Rio de Janeiro 225453-900, Brazil, e-mail: lodiaz@mat.puc-rio.br

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The example in [4] shows that this last requirement is too restrictive to be generic. For instance, this compatibility of hyperbolic structures implies that all saddles in a *transitive set* (the set is the closure of the orbit of some point of it) of an Axiom A diffeomorphism have the same *index* (dimension of the unstable bundle). In fact, the spectral decomposition of the limit set of Axiom A diffeomorphisms (see the precise result below) implies that any transitive set is contained in a hyperbolic transitive set.

After Abraham-Smale's construction new sort of examples of C^1-robustly non-Axiom A diffeomorphisms were obtained. First, [36] strengths the ideas in [4] to get robustly non-Axiom A diffeomorphisms in the three dimensional torus $\mathbb{T}^3$. Later, for closed manifolds of dimension three or higher, [35, 22, 7] provided examples of *robustly non-hyperbolic transitive diffeomorphisms*: the diffeomorphisms have a dense orbit in the whole manifold (thus the limit set is the whole ambient) and hyperbolic saddles of different indices. In the same spirit, [17, 18] showed that *heterodimensional cycles* (see the definition below) yield open sets of diffeomorphisms with transitive sets containing saddles of different indices. Note that the existence of saddles with different indices in the same transitive set Λ prevents the Axiom A property: by the comment above, there is a transitive hyperbolic set Σ containing Λ, hence all the saddles of Σ (thus of Λ) have the same index, a contradiction.

Note that, in dimension two, the C^1-density of Axiom A diffeomorphisms is an open problem. Newhouse's construction (see Sect. 3) implies that Axiom A diffeomorphisms are not dense in $\mathrm{Diff}^r(M)$, $r \geq 2$ and $\dim(M) \geq 2$. Finally, Axiom A diffeomorphisms (in fact, Morse-Smale) are open and dense in dimension one (any C^r-topology), see [31].

The construction in [4] provides hyperbolic sets whose invariant manifolds have robust non-transverse intersections. In this note, we give a framework for this construction, the so-called *co-index one heterodimensional cycles,* and state some consequences from the existence of robust cycles. Note first that non-transverse intersections of invariant manifolds are associated to hyperbolic sets of saddle-type. In the case of surface diffeomorphisms, the leaves of these invariant sets have dimension one and thus non-transverse intersections mean homoclinic and/or heteroclinic tangencies associated to hyperbolic sets. We illustrate the higher dimensional case considering the three-dimensional one. In that case, the invariant manifolds of hyperbolic sets of saddle-type may have either dimension one or two. Thus one needs to consider the occurrence of intersections between one-dimensional leaves. Such intersections are necessarily non-transverse (the sum of the dimensions of these leaves is $2 < 3 = \dim(M)$). The construction in [4] shows that these non-transverse intersections may be robust, leading to the notion of *robust heterodimensional cycle*.

A crucial point in [4] is the construction of a hyperbolic set Γ whose unstable manifold has dimension strictly greater than the dimension of its unstable bundle. Clearly, transitive Anosov diffeomorphisms are hyperbolic examples of this configuration. So a natural question is how to obtain this sort of sets in the non-Axiom A case. For example, the unfolding of very simple heterodimensional cycles yield the phenomenon of *jump of the topological dimension of invariant manifolds*: Assume

that the indices of the saddles P and Q in the cycle are u and $u+1$, then the closure of the u-dimensional unstable manifold of P contains the $(u+1)$-dimensional unstable manifold of Q. Thus, in some sense, the saddle P behaves simultaneously as a saddle of index u and $u+1$. This property is in the core of the notion of *blender* introduced in [7].

Roughly, a blender is a hyperbolic set whose embedding in the ambient manifold verifies some geometric properties, whose effect is that, as in the Abraham-Smale example, its unstable manifold behaves as a manifold of higher dimension. In this note blenders appear associated to *heterodimensional cycles* related to saddles. Note that, by Kupka-Smale's theorem, heterodimensional cycles associated to saddles occur in the complement of a residual set of diffeomorphisms, thus they never are robust. The key point here is that cycles associated to saddles generate non-trivial hyperbolic sets (corresponding to blenders) having different indices and related by C^1-robust heterodimensional cycles.

1.2 Basic Definitions

Given a diffeomorphism defined on a closed manifold, $f: M \to M$, a compact f-invariant subset Λ_f of M is *hyperbolic* if there is a Df-invariant splitting $T_{\Lambda_f} M = E^s \oplus E^u$ over Λ_f such that E^s and E^u are uniformly contracting and expanding. Every hyperbolic set Λ_f has a *continuation*: any diffeomorphism g close to f has a hyperbolic set Λ_g close to Λ_f with the same dynamics (there is a homeomorphism $h: \Lambda_f \to \Lambda_g$ with $g \circ h = h \circ f$). If Λ_f is hyperbolic and transitive then the dimensions of fibers E^u_x of the unstable bundle do not depend on $x \in \Lambda_f$. Then the dimension of the unstable bundle of Λ_f is its *index*.

A diffeomorphism f is *Axiom A* if its limit set $L(f)$ is hyperbolic and equal to the closure of its periodic points. In this case, the *spectral decomposition theorem*, [25], claims that $L(f)$ is the disjoint union of finitely many transitive sets Λ_i, called *basic sets.* Each basic set is a *homoclinic class*. Recall that the *homoclinic class* $H(P, f)$ of a hyperbolic periodic point P of f is the closure of the transverse intersections of the invariant manifolds (stable and unstable) of the orbit of P. Homoclinic classes are transitive sets and the saddles of the same index as P in $H(P, f)$ are dense in the class. Homoclinic classes may fail of being hyperbolic (we will see examples of that in this paper).

An Axiom A diffeomorphism f has a *cycle* if there are basic sets $\Lambda_{i_1}, \ldots, \Lambda_{i_n}$ of the spectral decomposition of the limit set of f such that $W^u(\Lambda_{i_k}) \cap W^s(\Lambda_{i_{k+1}}) \neq \emptyset$, for all $k = 1, \ldots, n$, where $i_{n+1} = i_1$. Here $W^u(\Lambda)$ and $W^s(\Lambda)$ stand for the unstable and stable manifolds of the hyperbolic set Λ.

A diffeomorphism f has a *heterodimensional cycle* associated to the hyperbolic sets Γ_f and Σ_f of f if the indices of Γ_f and Σ_f are different, the stable manifold of Γ_f meets the unstable manifold of Σ_f and the same holds for the stable manifold of Σ_f and the unstable manifold of Γ_f (in Fig. 1 there is depicted a heterodimensional cycle associated to a pair of saddles). The heterodimensional cycle has *co-index*

one if $\text{index}(\Sigma_f) = \text{index}(\Gamma_f) \pm 1$. Heterodimensional cycles can only occur in dimensions greater than or equal to three and heterodimensional cycles in dimension three have co-index one.

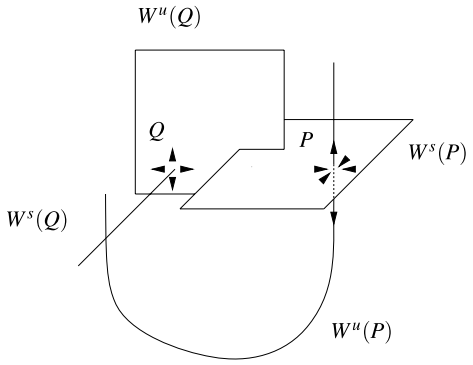

Fig. 1 A heterodimensional cycle

Finally, a heterodimensional cycle of f associated to Γ_f and Σ_f is C^r*-robust* if there is a C^r-neighborhood $\mathscr{U}$ of f such that every diffeomorphism $g \in \mathscr{U}$ has a heterodimensional cycle associated to the continuations Γ_g and Σ_g of Γ_f and Σ_f.

Recall that generically the invariant manifolds of hyperbolic periodic points are in general position (i.e., these invariant manifolds either are disjoint or have a non-empty transverse intersection). Therefore robust cycles must be associated to some non-trivial hyperbolic sets. Finally, diffeomorphisms f with robust heterodimensional cycles cannot satisfy (stably) the Axiom A condition. This follows by contradiction noting that (after an arbitrarily small perturbation) the robust cycle configuration gives limit points z whose ω and α-limits are contained in Γ_f and Σ_f, or vice-versa. By f-invariance and transitivity, both sets Γ_f and Σ_f are contained in the same basic set of $L(f)$. In particular, the unstable bundles of Γ_f and Σ_f have the same dimension, which is a contradiction.

1.3 Robust Cycles at Heterodimensional Cycles

Following the definition of robust heterodimensional cycle, a diffeomorphism f has a C^r*-robust homoclinic tangency* if there is a C^r-neighbourhood $\mathscr{U}$ of f such that any $g \in \mathscr{U}$ has a hyperbolic set Λ_g whose invariant manifolds have non-transverse intersections. Newhouse proved in [27] that homoclinic tangencies of C^2-diffeomorphisms of surfaces yield C^2-robust tangencies: any C^2-diffeomorphism f with a homoclinic tangency associated to a saddle P_f is in the closure of diffeomorphisms g with C^2-robust homoclinic tangencies. The occurrence of C^1-robust tangencies

for surface diffeomorphisms is an open problem. We will discuss this phenomenon in Sect. 3.

A first question is whether a situation similar to the one in [27] holds for heterodimensional cycles (i.e., heterodimensional cycles yield robust ones):

Question 1. Let f be a diffeomorphism with a heterodimensional cycle (associated to a pair of saddles). Does every C^1-neighborhood of f contain diffeomorphisms with C^1-robust heterodimensional cycles?

There is the following partial positive answer to this question:

Theorem 2 (Bonatti-D., [10]). *Let f be a C^1-diffeomorphism having a co-index one cycle associated to a pair of hyperbolic saddles. Then there are diffeomorphisms arbitrarily C^1-close to f having robust (heterodimensional) co-index one cycles.*

This theorem extends the results in [18] proving that co-index one cycles satisfying some natural geometrical conditions generates robustly non-hyperbolic transitive sets. Suppose that the saddles in the cycle have indices u and $(u+1)$. The main step in [18] is to check that, after a perturbation, the closure of the unstable manifold of the saddle of index u in the cycle contains the unstable manifold of the saddle of index $(u+1)$ and this property is robust. This feature corresponds to the hyperbolic set whose unstable manifold has dimension strictly greater than its index in [4] and it is a reformulation of the *distinctive property of blenders* in [14, Lemma 6.6]. As we will see in Sect. 3, this dimension property plays a role analogous to the *thick hyperbolic sets* in Newhouse's construction of C^2-robust homoclinic tangencies. In fact, we like to view Theorem 2 as a translation to the C^1-context and for heterodimensional cycles of Newhouse's result (homoclinic tangencies of C^2-diffeomorphisms yield robust tangencies).

Related to Theorem 2, we note that the phenomenon of robust cycles holds open and densely for the known examples of C^1-robustly non-Axiom A diffeomorphisms. First, the diffeomorphism in [4, 36] have robust cycles by construction. Second, the diffeomorphisms in [35, 22, 7] are robustly non-hyperbolic and robustly transitive. By [3] and [20, Connecting lemma], densely, there are saddles of consecutive indices related by heterodimensional cycles. Hence co-index one cycles occur densely and Theorem 2 implies the assertion.

As in dimension three heterodimensional cycles have co-index one, the following holds:

Corollary 3. *Every diffeomorphism f defined on a 3-manifold with a heterodimensional cycle associated to a pair of hyperbolic saddles belongs to the C^1-closure of the set of diffeomorphisms having C^1-robust heterodimensional cycles.*

In Sect. 4, we will review some key ingredients of the proof of Theorem 2: quotient dynamics and induced one-dimensional iterated function systems and model blenders.

1.4 Questions and Consequences

In view of the previous considerations, it is natural to ask how generally robust cycles appear for diffeomorphisms far from hyperbolic ones:

Question 4. Let M be closed manifold with $\dim(M) \geq 3$. Does it exist a C^1-open and dense subset $\mathscr{O} \subset \mathrm{Diff}^1(M)$ such that every $f \in \mathscr{O}$ either verifies the Axiom A and the no-cycles condition or has a C^1-robust heterodimensional cycle?

Actually, this question is a stronger version of the following conjecture due to Palis and proved for surface diffeomorphisms by Pujals and Sambarino in [33] (note that surface diffeomorphisms do not display heterodimensional cycles).

Conjecture 5 (Palis, [28]). Every diffeomorphism in $\mathrm{Diff}^1(M)$ can be C^1-approximated either by an Axiom A diffeomorphism or by a diffeomorphism with a homoclinic tangency or a heterodimensional cycle.

We will give positive answer to Question 4 in the special case of *tame diffeomorphisms*, (roughly, those having finitely many homoclinic classes), see Theorem 7 in Sect. 2.

Concerning Question 1, a natural strategy for solving it is to see that heterodimensional cycles yield secondary bifurcations corresponding to co-index one cycles. However, while the arguments in the proof of Theorem 2 are semi-local (the dynamics in a neighborhood of the saddles and of some heteroclinic orbits in the cycle), the higher co-index case seems to involve global dynamical ingredients. On the other hand, the approximation of heterodimensional cycles by co-index one cycles is true for robust cycles:

Corollary 6. *Every diffeomorphism with a C^1-robust heterodimensional cycle is C^1-approximated by diffeomorphisms with C^1-robust co-index one cycles.*

This corollary follows from Theorem 2, the properties of homoclinic classes of C^1-generic diffeomorphisms[1], and [20, Connecting Lemma]. First, by [15, 6, 3], there is a residual subset of $\mathrm{Diff}^1(M)$ such that, for diffeomorphisms in that residual subset, every non-disjoint homoclinic classes coincide and the indices of the saddles in any homoclinic class form an interval in $\mathbb{N}$. [20, Connecting Lemma] now implies that any generic f with a homoclinic class with saddles P_f and Q_f of different indices is approximated by diffeomorphisms g with a cycle associated to P_g and Q_g.

To prove now Corollary 6, consider a C^1-open set $\mathscr{U}$ of diffeomorphisms f with robust cycles associated to hyperbolic sets Γ_f and Σ_f of indices p and q, $p < q$. After a C^1-perturbation, one can assume that Γ_f and Σ_f are contained in the homoclinic classes of saddles P_f and Q_f of indices p and q. Using the robust cycle one can assume that these homoclinic classes are non-disjoint. Thus these classes coincide and contain saddles of indices $p, p+1, \ldots, q$. The Connecting Lemma now allows us to create a cycle associated to saddles of consecutive indices, obtaining a co-index one cycle. Corollary 6 now follows from Theorem 2.

[1] By C^1-*generic* diffeomorphisms we mean diffeomorphisms forming a residual subset of $\mathrm{Diff}^1(M)$.

2 Cycles and Non-hyperbolic Tame Dynamics

We now obtain some consequences of Theorem 2 and give a partial positive answer to Question 4 in the *tame setting.* We begin with some definitions.

2.1 Setting

The *chain recurrent set* of a diffeomorphism f, denoted by $R(f)$, is the set of points x such that, for every $\varepsilon > 0$, there is a closed ε-pseudo orbit $x = x_0, x_1, \ldots, x_n = x$, $d(f(x_i), x_{i+1}) < \varepsilon$, joining x to itself. The chain recurrent set is closed and contains the limit set. Two points x and y are in the same *chain recurrence class* if, for every $\varepsilon > 0$, there are ε-pseudo orbits going from x to y and vice-versa.

The fundamental theorem of dynamics, [16], says that the dynamics of the chain recurrent set is *stratified*: there is a continuous Liapunov function $L : M \to \mathbb{R}$ such that: (1) $L(f(x)) \leq L(x)$ and $L(f(x)) = L(x)$ if, and only if, $x \in R(f)$; (2) L is constant in the chain recurrence classes, and (3) $L(R(f))$ is a totally disconnected compact subset of $\mathbb{R}$. Using this Liapunov function one gets that each chain recurrence class has a basis of *filtrating neighbourhoods,* for details see, for instance, [2, Proposition 2.4]. Recall that U is a *filtrating set* if there are a pair of compact sets A and B such that $U = A \cap B$, $f(A) \subset \text{int}(A)$ (A is a trapping region for f), and $f^{-1}(B) \subset \text{int}(B)$ (that is, B is a trapping region for f^{-1}). A *filtrating neighborhood* of a chain recurrence class $\mathscr{C}(f)$ of f is a neighborhood of $\mathscr{C}(f)$ which is a filtrating set.

A diffeomorphism f is called *tame* if every chain recurrence class of it is robustly isolated. Denote by $\mathscr{T} = \mathscr{T}(M)$ the set of tame diffeomorphisms of the manifold M. For instance, Axiom A diffeomorphisms are tame ones, but there are tame diffeomorphisms which are not hyperbolic (for instance, the robustly transitive and non-hyperbolic diffeomorphisms in the examples above).

By [6], there is a residual set $\mathscr{G}$ of $\text{Diff}^1(M)$ of diffeomorphisms whose chain recurrence sets coincide with the closure of their hyperbolic periodic points and such that any chain recurrence class with a periodic point P is the homoclinic class of P. Moreover, isolated chain recurrence classes $\mathscr{C}(f)$ of $f \in \mathscr{G}$ are *robustly isolated*: there are neighborhoods $\mathscr{U}$ of f in $\text{Diff}^1(M)$ and O of the class $\mathscr{C}(f)$ in M such that, for every $g \in \mathscr{U}$, the intersection $R(g) \cap O$ is a unique chain recurrence class of g.

Let $\mathscr{T}_{\mathscr{G}} = \mathscr{T} \cap \mathscr{G}$. Then for every $f \in \mathscr{T}_{\mathscr{G}}$ the limit set of f is the disjoint union of finitely many homoclinic classes.

Using the Liapunov function L one gets a spectral decomposition for tame diffeomorphisms, replacing basic sets by chain recurrence classes. Moreover, for $f \in \mathscr{T}_{\mathscr{G}}$, the chain recurrence classes are homoclinic classes and the uniform hyperbolicity is replaced by weak hyperbolicity (uniform in dimension two, partial in dimension

three, and existence of a dominated splitting in higher dimensions)[2], see [1, 13]. Finally, the number of homoclinic classes of tame diffeomorphisms in $\mathscr{T}_{\mathscr{G}}$ is locally constant, see [1][3].

2.2 Tangencies, Heterodimensional Cycles, and Examples

For surface diffeomorphisms, homoclinic tangencies associated to saddles generate either sinks or sources (see, for example, [26]). For instance, a *dissipative* fixed saddle P of a diffeomorphism f (i.e., $f(P) = P$ and the Jacobian of $Df(P)$ is less than one) yields sinks. This generation of sinks/sources does not occur (necessarily) in higher dimensions. For example, consider a three dimensional diffeomorphism f with a normally hyperbolic surface N which is transversally expanding. Assume that the restriction $f_{|N}$ of f to N has a dissipative saddle $Q = f(Q)$ with a tangency. Note that the index of Q is two. See Fig. 2. The tangency of $f_{|N}$ generates sinks in N, but these sinks of the restriction to N correspond to saddles of index one of the global dynamics. Thus, in higher dimensions, homoclinic tangencies may generate saddles of different indices: in our example, a tangency associated to a saddle of index two generates saddles of index one.

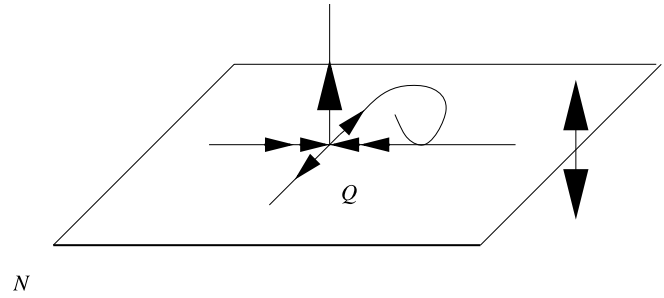

Fig. 2 Normally expanding manifold with a tangency

The comments above are the main reason because, in dimension three or higher, tame diffeomorphisms may exhibit homoclinic tangencies. However, these tangen-

[2] An f-invariant set Λ has a *dominated splitting* if the tangent bundle $T_\Lambda M$ over Λ splits into two Df-invariant bundles E and F, $T_\Lambda M = E \oplus F$, whose fibers E_x and F_x have constant dimensions, and there exists an integer $\ell \geq 1$ such that, for every point $x \in \Lambda$ and every pair of unit vectors $u \in E_x$ and $v \in F_x$ it holds that $\|Df^\ell(x)u\| \leq \frac{1}{2}\|Df^\ell(x)v\|$. The splitting $E \oplus F$ is *partially hyperbolic* if some of the bundles of the splitting is uniformly hyperbolic. For properties of dominated splittings we use in this note see, for example, [14, Appendix B].

[3] In fact, using the Liapunov function L, one gets a filtration $\{M_i\}_{i=0}^m$ (i.e., $M_i \subset M_{i+1}$, $M_0 = \emptyset$ and $M_m = M$, and $f(M_i)$ is contained in the interior of M_i) such that for each i the maximal invariant set of f in $(M_{i+1} \setminus M_i)$, $\Lambda_{i+1} = \cap_{i\in\mathbb{Z}} f^i(M_{i+1} \setminus M_i)$ is a homoclinic class of f.

cies are not *sectionally dissipative/expansive*. For simplicity, we explain this point in dimension three.

Consider a saddle P of a diffeomorphism f (assume that $f(P) = P$). This saddle P is *sectionally dissipative* (resp. *expansive*) if the modulus of the product of any pair of eigenvalues of $Df(P)$ is less (resp. greater) than one. For example, the saddle Q of index two in the example above is not sectionally expansive (the absolute value of the product of the two eigenvalues corresponding to the surface N is less than one). Note that, in dimension three, sectionally dissipative saddles have index one and sectionally expansive saddles have index two. Observe that there are saddles which are neither sectionally dissipative nor sectionally expansive.

A generalization of [26] is that homoclinic tangencies associated to sectionally dissipative (resp. expansive) saddles generate sinks (resp. sources), see [30, 34]. Since the number of homoclinic classes of a tame diffeomorphism is locally constant and sinks and sources are robust, tame diffeomorphisms cannot exhibit this sort of tangencies. However, there are tame diffeomorphism with homoclinic tangencies.

Reference [11] exhibits an open set $\mathscr{B}$ of non-hyperbolic transitive diffeomorphisms of $\mathrm{Diff}^1(\mathbb{T}^3)$ such that, for every $f \in \mathscr{B}$, $T(\mathbb{T}^3) = E^c \oplus E^u$ is a partially hyperbolic splitting of f such that E^c has dimension two and is undecomposable[4], non-hyperbolic, and volume contracting (roughly, the Jacobian of f in the central bundle is less than one), and E^u is uniformly expanding. Note that, by transitivity, the diffeomorphisms in $\mathscr{B}$ have a unique chain recurrence class (the whole manifold $\mathbb{T}^3$). Thus the set $\mathscr{B}$ consists of non-hyperbolic tame diffeomorphisms.

On the one hand, every diffeomorphism $f \in \mathscr{B}$ has saddles of indices one and two. Then there is a dense subset $\mathscr{D}$ of $\mathscr{B}$ such that every f in $\mathscr{D}$ has a homoclinic tangency associated to a saddle of index two. This follows from the robust transitivity, the Connecting Lemma, and the existence of saddles of index one with non-real eigenvalues (this is a consequence of the undecomposability of E^c). Since the central bundle E^c is volume contracting, the saddles of index one are not sectionally expansive. On the other hand, the robust transitivity, the Connecting Lemma, and the existence of saddles of indices one and two imply the existence of another dense subset $\mathscr{H}$ of $\mathscr{B}$ of diffeomorphisms having heterodimensional cycles.

Let us observe that there are non-hyperbolic tame diffeomorphisms which do not exhibit homoclinic tangencies. For instance, [22] exhibits an open set $\mathscr{M}$ of non-hyperbolic transitive diffeomorphisms of $\mathrm{Diff}^1(\mathbb{T}^3)$ having a partially hyperbolic splitting $T(\mathbb{T}^3) = E^{ss} \oplus E^c \oplus E^{uu}$ with three one dimensional bundles such that E^{ss} is uniformly contracting, E^{uu} is uniformly expanding, and E^c is non-hyperbolic. As above, by transitivity, the diffeomorphisms in $\mathscr{M}$ are tame (the whole $\mathbb{T}^3$ is the only chain recurrence class). Also as above, the diffeomorphisms contain saddles of indices one and two and, by the Connecting Lemma, there is a dense subset of $\mathscr{M}$ of diffeomorphisms with heterodimensional cycles. However, the splitting $E^{ss} \oplus E^c \oplus E^{uu}$ prevents the existence of homoclinic tangencies. This can be seen as follows. On the one hand, the angles between the bundles of a dominated splitting are uniformly bounded from below. On the other hand, a homoclinic tangency yields

[4] *Undecomposable* means that E^c does not admit any (non-trivial) dominated splitting.

saddles such that the angles between their stable and unstable bundles E^s and E^u are close to zero. Since either $E^s = E^{ss} \oplus E^c$ (if the saddle has index one) or $E^u = E^c \oplus E^{uu}$ (if the saddle has index two) this gives a contradiction.

After these motivations, we are ready to state our next result, claiming the occurrence of robust heterodimensional cycles in the setting of non-hyperbolic tame diffeomorphisms:

Theorem 7 (Bonatti-D, [10]). *There is an open and dense subset $\mathscr{O}$ of the set $\mathscr{T}$ of tame diffeomorphisms such that every $f \in \mathscr{O}$ is either hyperbolic* (*Axiom A plus the no-cycles condition*) *or has a C^1-robust heterodimensional cycle.*

We summarize Theorem 7 and the discussion above as follows: non-hyperbolic tame diffeomorphisms always yield robust cycles and tame diffeomorphisms with homoclinic tangencies always yield heterodimensional cycles, while the converse is not true in general.

3 Robust Homoclinic Tangencies, Non-dominated Dynamics, and Heterodimensional Cycles

The main difference between Question 4 and Conjecture 5 is that the conjecture involves, besides heterodimensional cycles, homoclinic tangencies. We now comment the role of homoclinic tangencies for C^1-diffeomorphisms. First, there are not known examples of surface diffeomorphisms with C^1-robust homoclinic tangencies (recall the definition in Sect. 1.3). Moreover, robust homoclinic tangencies in surfaces yield robustly non-dominated dynamics: the homoclinic class of the saddle involved in the tangency does not admit any dominated splitting. Finally, robustly non-dominated dynamics is the main source of robust instability of diffeomorphisms.

We also observe that the main known constructions of C^1-robustly non-dominated dynamics (in dimension three or higher) yield heterodimensional cycles and involve the notion of blender, [8, 9, 19]. These systems also yield C^1-*Newhouse's coexistence phenomenon* (existence of a C^1-open set $\mathscr{N}$ and a residual subset $\mathscr{N}$ of it formed by diffeomorphisms having infinitely many sinks or sources). There is also the construction in [5] of three dimensional diffeomorphisms with C^1-robust tangencies using derived from Plykin diffeomorphisms. Thus a key question is to decide whether there are diffeomorphisms with C^1-robust homoclinic tangencies (or with robustly non-dominated dynamics) far from the ones having heterodimensional cycles (of course, this is related to the discussion in Sect. 2). As surface diffeomorphisms do not display heterodimensional cycles, the simplest version of this question concerns C^1-robust tangencies of surface diffeomorphisms.

This last problem is closely related to Smale's conjecture of C^1-density of hyperbolic dynamics for surface diffeomorphisms (this conjecture remains open), see [40]. For a discussion on the current state of this conjecture we refer to [2], where it is proved that there are two sort of obstructions for the C^1-density of hyperbolicity: persistence of infinitely many hyperbolic homoclinic classes and existence of a

single homoclinic class with robust tangencies. The discussion here is related to the second obstruction.

In the setting of C^2-surface diffeomorphisms, Newhouse constructed diffeomorphisms with robust homoclinic tangencies and stated that homoclinic tangencies yield C^2-robust tangencies, see [24, 27] and [34, 30] for generalizations to higher dimensions. These results rely on the construction of *thick hyperbolic sets.*

A key ingredient in [24] is the notion of *thickness* $\tau(K)$ of a Cantor set K of the real line $\mathbb{R}$ (a kind of fractal dimension, see [29, Chap. 4] for details). The *Gap Lemma* ([29, Page 63]) claims that if two Cantor sets K_1 and K_2 of $\mathbb{R}$ satisfy $\tau(K_1)\tau(K_2) > 1$ then either $K_1 \cap K_2 \neq \emptyset$ or a Cantor set is contained in a *gap* of the other one (a gap of a Cantor set is a connected component of its complement). A crucial step in [27] is that every C^2-diffeomorphism f with a homoclinic tangency (say associated to a saddle P_f) generates diffeomorphisms g (close to f) with *thick hyperbolic sets* Λ_g contained in the homoclinic class of the continuation P_g of P_f for g: the Cantor sets $\Lambda_g^s = \Lambda_g \cap W^s_{loc}(P_g)$ and $\Lambda_g^u = \Lambda_g \cap W^u_{loc}(P_g)$ verify $\tau(\Lambda_g^s)\tau(\Lambda_g^u) > 1$.

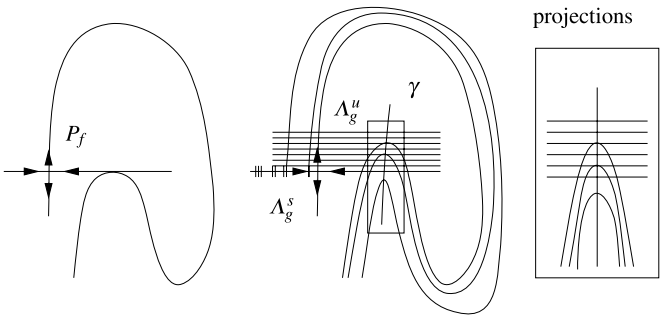

Fig. 3 C^2-Robust homoclinic tangencies

To obtain homoclinic tangencies associated to Λ_g one considers a curve γ (called *curve of tangencies*) containing the initial homoclinic tangency and projects the Cantor set Λ_g^s (resp. Λ_g^u) to γ along the stable (resp. unstable) leaves. This gives a pair of Cantor sets in the curve γ with the same thickness as Λ_g^s and Λ_g^u. Thus these Cantor sets verify the Gap Lemma. The geometric configuration implies that each Cantor set cannot be contained in a gap of the other one. The Gap Lemma now guarantees that these sets have non-empty intersection. Finally, each intersection corresponds to a homoclinic tangency of Λ_g. Figure 3 illustrates this construction.

The final (and essential) ingredient of Newhouse's construction is that, in the C^2-case, the property of having a thick hyperbolic set is open: for every h which is C^2-close to g, the continuation Λ_h of Λ_g is a thick hyperbolic set. This allows to repeat the previous construction for h close to g, getting C^2-robust homoclinic tangencies.

We point out that the thickness estimates involve distortion properties which only hold in the C^2-topology. [41] showed that the arguments in the previous construction

cannot be carried out to the C^1-topology: hyperbolic sets Λ_f of C^1-generic diffeomorphisms f have zero thickness (with the notation above, $\tau(\Lambda_f^s)\tau(\Lambda_f^u) = 0$). Moreover, Moreira recently presented evidences showing that hyperbolic sets of C^1-diffeomorphisms cannot exhibit robust tangencies, [23]. These results suggest that C^1-surface diffeomorphisms do not display robust tangencies. Therefore the occurrence of robust heterodimensional cycles is the only known source for C^1-robust non-hyperbolic dynamics. This suggests that the answers to Question 4 and Conjecture 5 should be both positive.

We close this discussion noting that the topological dimension property of blenders (the dimension of the unstable manifold of the blender is greater than its index) is a C^1-robust property. One can think of this property as a C^1-version of the thick hyperbolic sets in the heterodimensional setting. As in Newhouse's construction, this property is used for obtaining robust heterodimensional cycles (see Sect. 4.2).

4 Ingredients of the Proof of Theorem 2

To simplify the discussion of the proof of Theorem 2, we will assume that the dimension of the manifold is three and that the diffeomorphism f has a cycle associated to saddles $P = f(P)$ and $Q = f(Q)$ of indices one and two, respectively. The details of the proof can be found in [10].

We first consider a simple class of cycles, called *cycles with real multipliers,* such that the eigenvalues of the derivatives of $Df(P)$ and $Df(Q)$ are all real and positive and different in modulus. The first step (involving properties of homoclinic classes of C^1-generic diffeomorphisms) is to see that diffeomorphisms with heterodimensional cycles are approximated by diffeomorphisms with heterodimensional cycles with real multipliers. Therefore it is enough to prove the theorem for such sort of cycles.

There are two main advantages of considering cycles with real multipliers: there is some partial hyperbolicity inherited from the saddles in the cycle and a relevant part of the dynamics can be reduced to the study of an iterated function system of the interval. We proceed to explain these ideas briefly.

Consider a periodic point (from now on, we assume fixed) of a diffeomorphism f such that the derivative $Df(S)$ has real eigenvalues λ, 1, and β, with $\lambda < 1 < \beta$. In this case, we say that S is a *saddle-node* of f and the tangent space T_SM splits into three Df-invariant directions $T_SM = E^{ss}(S) \oplus E^c(S) \oplus E^{uu}(S)$, where $E^{ss}(S)$ and $E^{uu}(S)$ are the strong stable and strong unstable bundles and $E^c(S)$ is the center one. The *strong stable manifold* $W^{ss}(S)$ of S is the unique one-dimensional f-invariant manifold tangent to $E^{ss}(S)$. The *strong unstable manifold* of S, $W^{uu}(S)$, is defined similarly. The saddle-node S has a *strong homoclinic intersection* if there is some point $X \in W^{ss}(S) \cap W^{uu}(S)$ such that $W^{ss}(S)$ and $W^{uu}(S)$ meet quasi-transversely at X (i.e., $T_XW^{ss}(S) \oplus T_XW^{uu}(S)$).

The proof of Theorem 2 for cycles with real multipliers has two steps: (i) these cycles yield saddle-nodes with strong homoclinic intersections, and (ii) these strong homoclinic intersections generate C^1-robust cycles. We shortly explain these steps.

4.1 Strong Homoclinic Intersections of Saddle-Nodes

Since the saddles P and Q in the cycle have real multipliers, there is a Df-invariant partially hyperbolic splitting with one-dimensional directions

$$T_X M = E^{ss}_X \oplus E^c_X \oplus E^{uu}_X, \quad X = P, Q.$$

We can assume (after a perturbation) that there are small neighborhoods U_P and U_Q of P and Q and local coordinates in these neighborhoods where f is linear and

$$E^{ss} = \mathbb{R} \times \{(0,0)\}, \qquad E^c = \{0\} \times \mathbb{R} \times \{0\}, \qquad E^{uu} = \{(0,0)\} \times \mathbb{R}.$$

The stable bundle of P is $E^s(P) = E^{ss}(P) \oplus E^c(P)$ and the unstable bundle of Q is $E^u(Q) = E^c(Q) \oplus E^{uu}(Q)$. We also have $E^{uu}(P) = E^u(P)$ and $E^{ss}(Q) = E^s(Q)$.

We select heteroclinic points $X \in W^s(P) \cap W^u(Q)$ and $Y \in W^u(P) \cap W^s(Q)$, and assume that the intersection at $X \in W^s(P) \cap W^u(Q)$ is transverse and the intersection at $Y \in W^u(P) \cap W^s(Q)$ is quasi-transverse.

We take small neighborhoods U_X and U_Y of X and Y, and numbers n and m with

$$f^n(U_X) \subset U_P, \qquad f^{-n}(U_X) \subset U_Q,$$
$$f^{-m}(U_Y) \subset U_P, \quad \text{and} \quad f^m(U_Y) \subset U_Q.$$

Consider *transition times* $t_{(q,p)} = 2n$ and $t_{(p,q)} = 2m$ and *transition maps* $\mathfrak{T}_{(p,q)} = f^{t_{(p,q)}}$ from U_P to U_Q and $\mathfrak{T}_{(q,p)} = f^{t_{(q,p)}}$ from U_Q to U_P defined on small neighborhoods U^-_Y of $f^{-m}(Y)$ and U^-_X of $f^{-n}(X)$. Using the local coordinates, we write

$$\mathfrak{T}_{(q,p)} = (T^s_{(q,p)}, T^c_{(q,p)}, T^u_{(q,p)}) \colon U^-_X \to U_P,$$
$$\mathfrak{T}_{(p,q)} = (T^s_{(p,q)}, T^c_{(p,q)}, T^u_{(p,q)}) \colon U^-_Y \to U_Q,$$

where

$$T^s_{(i,j)}, T^c_{(i,j)}, T^u_{(i,j)} \colon \mathbb{R} \to \mathbb{R}, \quad (i,j) = (p,q) \text{ or } (q,p).$$

After a new C^1-perturbation of f, we can assume that the cycle associated to P and Q is *affine*: the transition maps are affine, $T^s_{(i,j)}$ and $(T^u_{(i,j)})^{-1}$ are contractions, and $T^c_{(a,b)}$ and $T^c_{(b,a)}$ are isometries. In fact, as the central coordinate of the heteroclinic points $f^{-m}(Y)$ and $f^m(Y)$ are both zero, the map $T^c_{a,b}$ is linear. These properties follows using the partial hyperbolicity of $E^{ss} \oplus E^c \oplus E^{uu}$, increasing the transition times n and m, and considering perturbations throughout the segments of orbits $\{f^{-n}(X), \ldots, f^n(X)\}$ and $\{f^{-m}(Y), \ldots, f^m(Y)\}$.

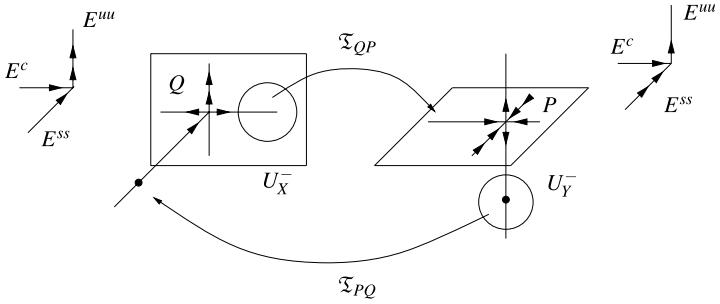

Fig. 4 Transitions

We take now a small neighborhood V of the saddles P and Q and of the orbits of the heteroclinic points X and Y. We say that V is a *neighborhood of the cycle*. The previous construction gives the *affine* dynamics of f in V. We next consider the unfolding of the cycle of f *via* a family of diffeomorphisms f_t preserving the affine structure of the cycle. Consider the one-parameter family of transitions $(\mathfrak{T}_{(p,q),\nu})_\nu$ from P to Q which in the local coordinates are of the form

$$\mathfrak{T}_{(p,q),\nu} = \mathfrak{T}_{(p,q)} + (0, \nu, 0).$$

To each small ν corresponds a local perturbation f_ν of f at the heteroclinic point Y. By construction, for every large ℓ and m, there is a small subset $U_{\ell,m}$ of U_X^- with

$$\begin{aligned} &\big(f_\nu^{\pi_{\ell,m}}\big)_{|U_{\ell,m}} = f^m \circ \mathfrak{T}_{(p,q),\nu} \circ f^\ell \circ \mathfrak{T}_{(q,p)} \colon U_{\ell,m} \to U_Q, \\ &\pi_{\ell,m} = \ell + t_{(q,p)} + m + t_{(p,q)}. \end{aligned}$$

Next, for each pair of large ℓ and m, we find a parameter $\nu = \nu_{\ell,m}$, $\nu_{\ell,m} \to \infty$ as $\ell, m \to \infty$, such that f_ν has a periodic point $R_{\ell,m}$ of period $\pi_{\ell,m}$. By construction, in the set V, the diffeomorphisms f_ν keep invariant the planes parallel to $\mathbb{R} \times \{0\} \times \mathbb{R}$ and act hyperbolically on these planes. We consider the quotient dynamics of f_ν by this family of planes, obtaining a one-dimensional map. Periodic points of this quotient dynamics correspond to periodic points of f_ν and the derivative of the quotient map is the derivative in the central direction. We next detail this point.

Assume that $X^- = f^{-n}(X) = (0, 1, 0)$ and $X^+ = f^n(x) = (0, -1, 0)$. So $T^c_{(q,p)}(1) = -1$. Assume that $T^c_{(p,q)}(y) = y$ (the case $T^c_{(p,q)}(y) = -y$ is similar).

Suppose that the eigenvalues of P and Q corresponding to the central direction are λ and β, $0 < \lambda < 1 < \beta$. Fix large ℓ and m and let

$$\nu_{\ell,m} = \beta^{-m} + \lambda^\ell, \qquad \nu_{\ell,m} \to 0 \quad \text{as} \quad \ell, m \to \infty.$$

Therefore, by definition of $\nu_{\ell,m}$ and by construction,

$$\beta^m(-\lambda^\ell + \nu_{\ell,m}) = 1, \qquad T^c_{(q,p)}(1) = -1, \qquad T^c_{(p,q),\nu_{\ell,m}}(y) = y + \nu_{\ell,m}.$$

These choices imply that 1 is a fixed point of the quotient dynamics:

$$\begin{aligned}\beta^m \circ T^c_{(p,q),\nu_{\ell,m}} \circ \lambda^\ell \circ T^c_{(q,p)}(1) &= \beta^m \circ T^c_{(p,q),\nu_{\ell,m}} \circ \lambda^\ell(-1)\\ &= \lambda^m \circ T^c_{(p,q),\nu_{\ell,m}}(-\lambda^\ell) = \beta^m(-\lambda^\ell + \nu_{\ell,m}) = 1.\end{aligned}$$

As $f_{\ell,m} = f_{\nu_{\ell,m}}$ preserves the E^{ss}, E^{uu}, and E^c, the hyperbolicity of E^{ss} and E^{uu} implies that the map $f^m \circ \mathfrak{T}_{(p,q),\nu_{\ell,m}} \circ f^\ell \circ \mathfrak{T}_{(q,p)}$ has a fixed point $R_{\ell,m} = (r^s_{\ell,m}, 1, r^u_{\ell,m})$ in $U_{\ell,m}$ with $|r^{u,s}_{\ell,m}| \to 0$ as $\ell, m \to \infty$ (i.e., as $\nu_{\ell,m} \to 0$). Therefore $R_{\ell,m}$ is a periodic point of $f_{\ell,m}$ with period $\pi_{\ell,m}$, E^{ss} and E^{uu} are hyperbolic directions of $R_{\ell,m}$, and the derivative of $Df^{\pi_{\ell,m}}_{\ell,m}(R_{\ell,m})$ in the central direction is $\kappa_{\ell,m} = \beta^m\lambda^\ell$. Considering now the multiplication by factor $\kappa^{-1/\pi_{\ell,m}}_{\ell,m}$ along the orbit of $R_{\ell,m}$ one has that $R_{\ell,m}$ is a saddle-node.

It remains to see that the saddle-node $R_{\ell,m}$ can be chosen with a strong homoclinic intersection. For that it suffices to see that we can choose λ and β such that there are natural numbers i and j, $i \neq \ell$ and $j \neq m$, such that

$$\beta^j \circ T^c_{(p,q),\nu_{\ell,m}} \circ \lambda^i \circ T^c_{(q,p)}(1) = 1.$$

In other words, the point 1 is a fixed point of the quotient iterated function system with two different periodic itineraries. Observe that the (strong) unstable and stable manifolds of $R_{\ell,m}$ contain the disks $\Delta^u = \{(r^s_{\ell,m}, 1)\} \times [-1, 1]$ and $\Delta^s = [-1, 1] \times \{(1, r^u_{\ell,m})\}$, respectively. By construction and the choice of i and j, we have that

$$\begin{aligned}\{(a, 1)\} \times [-1, 1] &\subset f^i \circ \mathfrak{T}_{(p,q),\nu_{\ell,m}} \circ f^j \circ \mathfrak{T}_{(q,p)}(\Delta^u)\\ &= f^{i+t_{(p,q)}+j+t_{(q,p)}}_{\ell,m}(\Delta^u) \subset W^{uu}(R_{\ell,m}, f_{\ell,m}),\end{aligned}$$

for some a. Thus $W^{uu}(R_{\ell,m}, f_{\ell,m})$ meets the disk Δ^s, thus it intersects $W^{ss}(R_{\ell,m}, f_{\ell,m})$. As $(i, j) \neq (\ell, m)$ this intersection point is not $R_{\ell,m}$, proving our assertion.

4.2 Model Blenders

We begin this section by introducing a simple model of blender in dimension three. Consider a map ϕ defined in the $\mathbb{XZ}$ plane having an affine horseshoe in the square $[0, 1]^2$,

$$\phi(x, z) = \begin{cases}(\frac{1}{3}x, 3z), & (x, z) \in [0, 1] \times [0, 1/3],\\ (1 - \frac{1}{3}x, 3 - 3z), & (x, z) \in [0, 1], z \in [2/3, 1].\end{cases}$$

We fix $\sigma \in (1, 2)$ and define the one-parameter family of maps Φ_t in $[0, 1]^2 \times \mathbb{R}$ as follows:

$$\Phi_t(x,z,y)=\begin{cases}(\phi(x,z),\sigma y), & (x,z)\in[0,1]\times[0,1/3],\\ (\phi(x,z),\sigma y)+(0,0,t), & (x,z)\in[0,1]\times[2/3,1].\end{cases}$$

The maps Φ_t are depicted in Fig. 5.

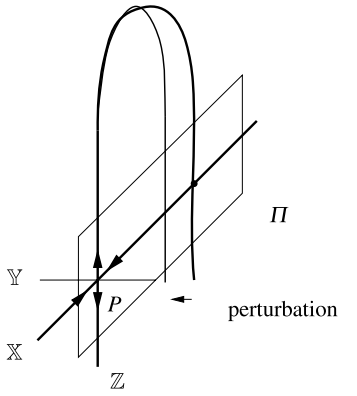

Fig. 5 The maps Φ_t and non-normally hyperbolic horseshoes

Note that Φ_0 has an affine horseshoe Λ_0 of index two in the square $[0,1]^2\times\{0\}$ and that the plane $\Pi=\mathbb{XZ}\times\{0\}$ is not normally hyperbolic. For each small t, we denote by Λ_t the continuation of Λ_0 for Φ_t. Since Π is not normally hyperbolic, Λ_t is not (necessarily) contained in Π for $t\neq 0$. Note that Λ_t is the homoclinic class of the saddle $P=(0,0,0)$.

The diffeomorphisms Φ_t verify the following property meaning that the one-dimensional stable manifold of P behaves (in some sense) as a two-dimensional one.

Proposition 8 ([12]). *Consider $t<0$ and let $s(t)=\frac{|t|}{\sigma-1}$. Then the stable manifold of P for Φ_t meets transversely any two disk of the form $\{a\}\times[0,1]\times[c,d]$, where $0\le a\le 1$ and $0\le c<d\le s(t)$, where $a\in\mathbb{X}$, $[0,1]\subset\mathbb{Z}$, and $[c,d]\subset\mathbb{Y}$.*

In fact, this proposition shows that the stable manifold of Λ_t meets every vertical disk crossing from the bottom to the top the cube $[0,1]^2\times[0,s(t)]$.

Proof. Note that since $\sigma\in(1,2)$, $s(t)=\frac{|t|}{\sigma-1}>|t|$ (this is the only place where this hypothesis is used). Consider the (partially bi-valuated) interval map g,

$$g\colon[0,s(t)]\to[0,s(t)],\qquad \begin{cases}g(x)=g_0(x)=\sigma x, & x\in[0,\frac{s(t)}{\sigma}]=I_0,\\ g(x)=g_1(x)=\sigma x+t, & x\in[\frac{t}{\sigma},s(t)]=I_1.\end{cases}$$

We claim that the orbit of any interval $J\subset[0,s(t)]$ meets the point t/σ. We consider $g_0(J)$ if $J\subset I_0$ and $g_1(J)$ if $J\subset I_1'=[s(t)/\sigma,s(t)]$. Note that if J is contained neither in I_0 nor in I_1' then it contains t/σ and there is nothing to prove. In this way, we get a family of intervals $J_i=g^i(J_0)$, $J_0=J$, such that either

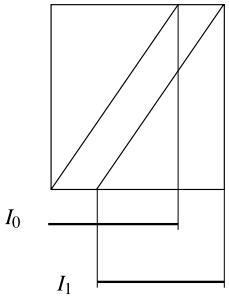

Fig. 6 The map g

$|J_i| = \sigma^i |J_0|$ or J_i contains t/σ. Since the lengths of I_0 and I_1' are finite and $\sigma > 1$, there is a first J_i containing t/σ.

To prove the proposition consider any disk $\Delta_0 = \{a_0\} \times [0, 1] \times J_0$, $J_0 \subset [0, s(t)]$. By definition of Φ_t, $\Phi_t(\Delta_0)$ contains a disk Δ_1 of the form $= \{a_1\} \times [0, 1] \times g(J_0)$. By the claim and arguing inductively, there is a first $k \geq 0$ such that $\Phi_t^k(\Delta)$ contains a vertical segment $V = \{a_k\} \times [0, 1] \times \{t/\sigma\}$ for some a_k. By definition of Φ_t, the set $\Phi_t(V)$ meets $[0, 1] \times \{(0, 0)\} \subset W^s(P, \Phi_t)$. This ends the proof of the proposition. □

We now explain how the construction above is used to get robust cycles in our setting. First, note that a diffeomorphism having a strong homoclinic intersection associated to a saddle-node in Sect. 4.1 can be perturbed to get a horseshoe as in the example above. Thus we can consider perturbations of this horseshoe verifying Proposition 8. Moreover, the property in Proposition 8 is robust (one needs to consider a reformulation considering cone-fields in the spirit of [7, Lemma 1.11]). The key point is that considering the saddle-node and its strong homoclinic intersection one can also obtain a saddle Q of index one whose one dimensional unstable manifold crosses the cube $[0, 1]^2 \times [0, s(t)]$. This implies that the stable manifold of Λ_t intersects the unstable manifold of Q. Using this fact, one gets the robust cycles.

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Hamiltonian Perturbations of Hyperbolic PDEs: from Classification Results to the Properties of Solutions

Boris Dubrovin

Abstract We begin with presentation of classification results in the theory of Hamiltonian PDEs with one spatial dimension depending on a small parameter. Special attention is paid to the deformation theory of integrable hierarchies, including an important subclass of the so-called integrable hierarchies of the topological type associated with semisimple Frobenius manifolds. Many well known equations of mathematical physics, such as KdV, NLS, Toda, Boussinesq etc., belong to this subclass, but there are many new integrable PDEs, some of them being of interest for applications. Connections with the theory of Gromov–Witten invariants and random matrices are outlined. We then address the problem of comparative study of singularities of solutions to the systems of first order quasilinear PDEs and their Hamiltonian perturbations containing higher derivatives. We formulate Universality Conjectures describing different types of critical behavior of perturbed solutions near the point of gradient catastrophe of the unperturbed one.

1 Introduction

The main subject of our research is the study of Hamiltonian perturbations of systems of hyperbolic[1] PDEs

$$u^i_t + A^i_j(u)u^j_x + \text{higher order derivatives} = 0, \quad i = 1, \dots, n.$$

(Here and below the summation over repeated indices will be assumed.) They can be obtained, in particular, by applying the procedure of *weak dispersion expansion*:

Boris Dubrovin
SISSA, via Beirut 2-4, 34014, Trieste, Italy and Steklov Mathematical Institute, Moscow, Russia, e-mail: dubrovin@sissa.it

[1] Always the strong hyperbolicity will be assumed, i.e., the eigenvalues of the $n \times n$ matrix $(A^i_j(u))$ are all real and pairwise distinct for all $u = (u^1, \dots, u^n)$ in the domain under consideration.

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starting from a system of PDEs

$$u^i_t + F^i(u, u_x, u_{xx}, \ldots) = 0, \quad i = 1, \ldots, n$$

with the analytic right hand side let us introduce *slow variables*

$$x \mapsto \epsilon x, \quad t \mapsto \epsilon t.$$

Expanding in ϵ one obtains, after dividing by ϵ a system of the above form

$$\frac{1}{\epsilon} F^i(u, \epsilon u_x, \epsilon^2 u_{xx}, \ldots) = A^i_j(u) u^j_x + \epsilon \left(B^i_j(u) u^j_{xx} + \frac{1}{2} C^i_{jk}(u) u^j_x u^k_x \right) + \cdots$$

assuming all the dependent variables are *slow*, i.e., the terms of the order $1/\epsilon$ vanish:

$$F^i(u, 0, 0, \ldots) \equiv 0, \quad i = 1, \ldots, n.$$

E.g., the celebrated Korteweg–de Vries (KdV) equation

$$u_t + u u_x + \frac{\epsilon^2}{12} u_{xxx} = 0 \tag{1}$$

is one of the most well known examples of such a weakly dispersive Hamiltonian PDE. Another class of examples comes from interpolated discrete systems. Let us consider the simplest example of Toda lattice: an infinite system of particles on the line with exponential interaction of neighbors. The equations of motion

$$\left.\begin{aligned} \dot{q}_n &= \tfrac{\partial H}{\partial p_n} \\ \dot{p}_n &= -\tfrac{\partial H}{\partial q_n} \end{aligned}\right\}, \quad n \in \mathbb{Z}$$
$$H = \sum_{n \in \mathbb{Z}} \frac{p_n^2}{2} + e^{q_n - q_{n-1}} \tag{2}$$

after the interpolation

$$\begin{aligned} q_{n+1} - q_n &= u(n\epsilon) \\ p_n &= v(n\epsilon) \end{aligned}$$

can be recast into the form (6) via the (formal) Taylor expansion

$$\begin{aligned} u_t &= \frac{1}{\epsilon} [v(x + \epsilon) - v(x)] = v_x + \frac{1}{2} \epsilon v_{xx} + \cdots \\ v_t &= \frac{1}{\epsilon} \left[e^{u(x)} - e^{u(x-\epsilon)} \right] = e^u u_x - \frac{1}{2} \epsilon \left(e^u \right)_{xx} + \cdots . \end{aligned} \tag{3}$$

Another class of infinite expansions comes from a nonlocal evolution. An example of Camassa–Holm equation

$$u_t - u_{txx} = \frac{3}{2}uu_x - \left[u_x u_{xx} + \frac{1}{2}uu_{xxx}\right] \tag{4}$$

illustrates the procedure. After the introduction of the slow variables $x \mapsto \epsilon x,\ t \mapsto \epsilon t$ we use the geometric series

$$\left(1 - \epsilon^2 \partial_x^2\right)^{-1} = 1 + \epsilon^2 \partial_x^2 + \epsilon^4 \partial_x^4 + \cdots$$

in order to rewrite the Camassa–Holm equation in the form (6):

$$u_t = \frac{3}{2}uu_x + \epsilon^2\left(uu_{xxx} + \frac{7}{2}u_x u_{xx}\right) + O(\epsilon^4). \tag{5}$$

Let us return back to the general setting. Loosely speaking the system of PDEs

$$u_t^i + A_j^i(u)u_x^j + \epsilon\left(B_j^i(u)u_{xx}^j + \frac{1}{2}C_{jk}^i(u)u_x^j u_x^k\right) + \cdots = 0, \quad i = 1, \ldots \tag{6}$$

depending on a small parameter ϵ will be considered as a Hamiltonian vector field on the "infinite dimensional manifold"

$$\mathcal{L}(M^n) \otimes \mathbb{R}[[\epsilon]] \tag{7}$$

where M^n is a n-dimensional manifold (in all our examples it will have topology of a ball) and

$$\mathcal{L}(M^n) = \left\{S^1 \to M^n\right\}$$

is the space of loops on M^n. The dependent variables

$$u = (u^1, \ldots, u^n) \in M^n$$

are local coordinates on M^n. In the expansion (6) the terms of order ϵ^k are *polynomials* of degree $k + 1$ in the derivatives $u_x, u_{xx}, \ldots$ where

$$\deg u^{(m)} = m, \quad m = 1, 2, \ldots.$$

The coefficients of these polynomials are smooth functions defined in every coordinate chart on M^n. Clearly the above gradation on the ring of polynomial functions on the jet bundle $J^\infty(M^n)$ does not depend on the choice of local coordinates. The systems of the form (6) will be assumed to be Hamiltonian flows

$$u_t^i = \{u^i(x), H\} = \sum_{k\geq 0} \epsilon^k \sum_{m=0}^{k+1} A_{k,m}^{ij}\left(u; u_x, \ldots, u^{(m)}\right)\partial_x^{k-m+1}\frac{\delta H}{\delta u^j(x)} \tag{8}$$

with respect to *local Poisson brackets*

$$\{u^i(x), u^j(y)\} = \sum_{k\geq 0} \epsilon^k \sum_{m=0}^{k+1} A^{ij}_{k,m}\Big(u(x); u_x(x), \dots, u^{(m)}(x)\Big)\delta^{(k-m+1)}(x-y) \tag{9}$$
$$\deg A^{ij}_{k,m}\Big(u; u_x, \dots, u^{(m)}\Big) = m$$

with *local Hamiltonians*

$$H = \sum_{k\geq 0} \epsilon^k \int h_k\Big(u; u_x, \dots, u^{(k)}\Big)\, dx \tag{10}$$
$$\deg h_k\Big(u; u_x, \dots, u^{(k)}\Big) = k.$$

Here $\delta(x)$ is the Dirac delta-function. The meaning of the delta-function and of its derivatives is clear from the explicit expression (8). The integral in (10) is understood in the sense of formal variational calculus, i.e., for a differential polynomial $h = h(u; u_x, \dots, u^{(m)})$ the integral

$$\int h(u; u_x, \dots, u^{(m)})\, dx$$

is the class of equivalence of h modulo the total x-derivative:

$$h(u; u_x, \dots, u^{(m)}) \sim h(u; u_x, \dots, u^{(m)}) + \partial_x\Big(f(u; u_x, \dots, u^{(m-1)}\Big)$$
$$\partial_x = \sum_{k\geq 0} u^{i\,(k+1)} \frac{\partial}{\partial u^{i\,(k)}}.$$

$\delta H/\delta u^j(x)$ is the Euler–Lagrange operator

$$\frac{\delta H}{\delta u^j(x)} = \frac{\partial h}{\partial u^j} - \partial_x \frac{\partial h}{\partial u^j_x} + \partial_x^2 \frac{\partial h}{\partial u^j_{xx}} - \cdots \quad \text{for } H = \int h\, dx.$$

The coefficients of the Poisson bracket and Hamiltonian densities will always be assumed to be differential polynomials. The antisymmetry and Jacobi identity for the Poisson bracket (9) are understood as identities for formal power series in ϵ. The Poisson bracket (9) defines a structure of a Lie algebra $\mathcal{G}_{\rm loc}$ on the space of all local functionals

$$\{F, G\} = \int \frac{\delta F}{\delta u^i(x)} A^{ij} \frac{\delta G}{\delta u^j(x)}\, dx$$
$$A^{ij} := \sum_{k\geq 0} \epsilon^k \sum_{m=0}^{k+1} A^{ij}_{k,m}\Big(u; u_x, \dots, u^{(m)}\Big)\partial_x^{k-m+1} \tag{11}$$
$$F = \sum_{k\geq 0} \epsilon^k \int f_k(u; u_x, \dots, u^{(k)})\, dx, \qquad G = \sum_{l\geq 0} \epsilon^l \int g_l(u; u_x, \dots, u^{(l)})\, dx$$

$$\deg f_k(u; u_x, \dots, u^{(k)}) = k, \qquad \deg g_l(u; u_x, \dots, u^{(l)}) = l.$$

The full ring of functions on the infinite dimensional manifold $\mathcal{L}(M^n) \otimes \mathbb{R}[[\epsilon]]$ is obtained by taking the suitably completed symmetric tensor algebra of $\mathcal{G}_{\mathrm{loc}}$.

Let us now introduce the class of "coordinate changes" on the infinite dimensional manifold $\mathcal{L}(M^n) \otimes \mathbb{R}[[\epsilon]]$. Define a *generalized Miura transformation*

$$\begin{aligned} u^i \mapsto \tilde{u}^i &= \sum_{k\geq 0} \epsilon^k F_k^i \left(u; u_x, \dots, u^{(k)}\right) \\ \deg F_k^i \left(u; u_x, \dots, u^{(k)}\right) &= k \\ \det \left(\frac{\partial F_0^i(u)}{\partial u^j}\right) &\neq 0. \end{aligned} \tag{12}$$

The coefficients $F_k^i(u; u_x, \dots, u^{(k)})$ are differential polynomials. It is easy to see that the transformations of the form (12) form a group.[2] The classes of evolution PDEs (6), local Poisson brackets (9) and local Hamiltonians (10) are invariant with respect to the action of the group of generalized Miura transformations. We say that two objects of our theory (i.e., two evolutionary vector fields of the form (6), two local Poisson brackets of the form (9), or two local Hamiltonians of the form (10)) are *equivalent* if they are related by a generalized Miura transformation.

Our main goal is the *classification* of Hamiltonian PDEs (6), (8) with respect to the above equivalence relation. We will also address the problem of selection of *integrable* Hamiltonian PDEs. Last but not least, we will study the general properties of *solutions* to Hamiltonian PDEs of the form (6), (8).

2 Towards Classification of Hamiltonian PDEs

The first step is the classification of local Poisson brackets (9) with respect to the action of the group of Miura-type transformations.

Theorem 1. *Under assumption*

$$\det \left(A_{0,0}^{ij}(u)\right) \neq 0 \tag{13}$$

any bracket of the form (9) *is equivalent to*

$$\left\{\tilde{u}^i(x), \tilde{u}^j(y)\right\} = \eta^{ij}\delta'(x-y), \quad \eta^{ij} = \eta^{ji} = \mathrm{const}, \quad \det(\eta^{ij}) \neq 0. \tag{14}$$

The *proof* of this theorem consists of two parts. The first part deals with the analysis of the *leading term* of the Poisson bracket. Setting $\epsilon \to 0$ one obtains

[2] To invert the transformation one has to solve the differential equation (12) for $u^1, \dots, u^n$. The solution in question is written as the formal WKB expansion.

again a Poisson bracket of a simpler form

$$\left\{u^i(x), u^j(y)\right\}^{[0]} = A^{ij}_{0,0}(u(x))\delta'(x-y) + A^{ij}_{0,1}(u(x); u_x(x))\delta(x-y). \quad (15)$$

Here the coefficient $A^{ij}_{0,1}(u; u_x)$ depends linearly on u_x. This is a so-called *Poisson bracket of hydrodynamic type* introduced in 1983 by B. Dubrovin and S.P. Novikov [21]. One of the main results of [21] says that, under the assumption (13) the leading term

$$g^{ij}(u) := A^{ij}_{0,0}(u) \quad (16)$$

is a (contravariant) Riemannian or pseudo-Riemannian metric of the curvature zero on the underlying manifold M^n; the second coefficient must have the form

$$A^{ij}_{0,1}(u; u_x) = \Gamma^{ij}_k(u)u^k_x, \quad \Gamma^{ij}_k(u) = -g^{is}(u)\Gamma^j_{sk}(u) \quad (17)$$

where $\Gamma^j_{sk}(u)$ are the Christoffel coefficients for the Levi-Civita connection for the metric $g^{ij}(u)$. Due to triviality of the topology of M^n one can choose a global system of flat coordinates for the metric

$$\tilde{u}^i = \tilde{u}^i(u), \quad \frac{\partial \tilde{u}^i}{\partial u^k}\frac{\partial \tilde{u}^j}{\partial u^l}g^{kl}(u) = \eta^{ij} = \text{const}.$$

In these coordinates the Poisson bracket (15) takes the form (14).

The second part of the proof is based on the deformation theory of the Poisson bracket (14). We may assume that the original Poisson bracket (9) has the form

$$\left\{u^i(x), u^j(y)\right\} = \eta^{ij}\delta'(x-y) + O(\epsilon).$$

The first correction is a 2-cocycle in the Poisson cohomology of the "manifold" $\mathcal{L}(M^n) \otimes \mathbb{R}[[\epsilon]]$ equipped with the Poisson bracket (14). This first correction can be eliminated by a "change of coordinates", i.e., by a generalized Miura transformation, *iff* this 2-cocycle is trivial. To complete the proof of Theorem 1 one has to use triviality of the Poisson cohomology in positive degrees in ϵ proved in [39] (see also [12]).

Corollary 2. *Any system of Hamiltonian PDEs for slow dependent variables satisfying the nondegeneracy assumption* (13) *can be reduced to the following standard form*

$$u^i_t = \eta^{ij}\partial_x \frac{\delta H}{\delta u^j(x)}, \quad i = 1, \ldots, n \quad (18)$$

with the Hamiltonian of the form (10)*. Two such systems are equivalent* iff *the Hamiltonians are related by a canonical transformation*

$$\begin{aligned} &H \mapsto H + \epsilon\{F, H\} + \frac{\epsilon^2}{2}\{F, \{F, H\}\} + \cdots, \\ &F = \sum_{k\geq 0} \epsilon^k \int f_k\left(u; u_x, \ldots, u^{(k)}\right) dx, \quad \deg f_k\left(u; u_x, \ldots, u^{(k)}\right) = k. \end{aligned} \tag{19}$$

In order to prove the second part of the corollary one has to use triviality in the positive degrees in ϵ of the first Poisson cohomology of the bracket (14). This implies that any canonical transformation close to identity must have the form

$$\begin{aligned} &u^i(x) \mapsto \tilde{u}^i(x) = u^i(x) + \epsilon\{F, u^i(x)\} + \frac{\epsilon^2}{2}\{F, \{F, u^i(x)\}\} + \cdots \\ &\{\tilde{u}^i(x), \tilde{u}^j(y)\} = \{u^i(x), u^j(y)\} = \eta^{ij}\delta'(x-y) \end{aligned} \tag{20}$$

with the generating Hamiltonian F of the above form polynomial in jets in every order in ϵ.

Example 3. The Riemann equation

$$v_t + vv_x = 0 \tag{21}$$

is a Hamiltonian system

$$v_t + \partial_x \frac{\delta H_0}{\delta v(x)} = 0$$

with the Hamiltonian

$$H_0 = \int \frac{v^3}{6}\, dx \tag{22}$$

and the Poisson bracket of the form (14):

$$\{v(x), v(y)\} = \delta'(x-y). \tag{23}$$

Any Hamiltonian perturbation of this equation of order ϵ^4 can be reduced to the following normal form parametrized by two arbitrary functions of one variable $c = c(u)$, $p = p(u)$:

$$\begin{aligned} &u_t + uu_x + \frac{\epsilon^2}{24}\left[2cu_{xxx} + 4c'u_xu_{xx} + c''u_x^3\right] \\ &\quad + \epsilon^4\Big[2pu_{xxxxx} + 2p'(5u_{xx}u_{xxx} + 3u_xu_{xxxx}) + p''(7u_xu_{xx}^2 + 6u_x^2u_{xxx}) \\ &\quad + 2p'''u_x^3u_{xx}\Big] = 0. \end{aligned} \tag{24}$$

The Hamiltonian has the form

$$H = \int \left[\frac{u^3}{6} - \epsilon^2\frac{c(u)}{24}u_x^2 + \epsilon^4 p(u)u_{xx}^2\right] dx. \tag{25}$$

Two such perturbations are equivalent iff the associated functional parameters $c(u)$, $p(u)$ coincide.

3 Deformation Theory of Integrable Hierarchies

We will now concentrate on the study of integrable hyperbolic systems

$$v_t^i + A_j^i(v)v_x^j = 0, \quad i = 1, \dots, n$$

and their Hamiltonian perturbations. The word 'hyperbolic' will stand for *strong hyperbolicity*, i.e., all eigenvalues of the matrix $(A_j^i(v))$, $v \in M^n$, will be assumed real and pairwise distinct. We will also consider the complex analytic situation where the eigenvalues of the matrix will be assumed to be distinct.

Let us first recall the main points of the theory of integrable hyperbolic PDEs.

Definition 4. A hyperbolic system

$$\begin{aligned} &v_t^i + A_j^i(v)v_x^j = v_t^i + \eta^{ij}\partial_x \frac{\delta H_0}{\delta v^j(x)} = 0 \\ &H_0 = \int h(v)\,dx, \qquad A_j^i(v) = \eta^{is}\frac{\partial^2 h(v)}{\partial v^s \partial v^j} \end{aligned} \tag{26}$$

is called integrable if the Lie algebra of first integrals F_0 of the form

$$F_0 = \int f(v)\,dx, \qquad \{H_0, F_0\} = 0 \tag{27}$$

possesses the following property of maximality: solutions $f = f(v)$ to the overdetermined system of equations

$$\frac{\partial^2 f}{\partial v^i \partial v^l}\eta^{ij}\frac{\partial^2 h}{\partial v^j \partial v^k} = \frac{\partial^2 f}{\partial v^i \partial v^k}\eta^{ij}\frac{\partial^2 h}{\partial v^j \partial v^l}, \quad k, l = 1, \dots, n \tag{28}$$

equivalent to (27) depend on the maximal number ($= n$) of arbitrary functions of one variable.

First integrals of an integrable system of hyperbolic PDEs form a maximal Abelian subalgebra in the Lie algebra $\mathcal{G}_{\text{loc}}$ of local Hamiltonians [25]. The Hamiltonian flow

$$v_s^i + B_j^i(v)v_x^j = v_s^i + \eta^{ij}\partial_x \frac{\delta F_0}{\delta v^j(x)}, \quad B_j^i(v) = \eta^{is}\frac{\partial^2 f(v)}{\partial v^s \partial v^j} \tag{29}$$

generated by any solution to (27) is an infinitesimal symmetry of the hyperbolic system (26):

$$\frac{\partial}{\partial s}\frac{\partial v^i}{\partial t} = \frac{\partial}{\partial t}\frac{\partial v^i}{\partial s}, \quad i = 1, \dots, n. \tag{30}$$

All these symmetries commute pairwise due to commutativity of the Lie algebra of conservation laws. Integrability of the Hamiltonian hyperbolic system (26) is equivalent to its diagonalizability (i.e., existence of *Riemann invariants*) [66]. Recall that the necessary and sufficient condition for diagonalizability is vanishing of the Haantjes tensor [44] in the case under consideration written in the form

$$\begin{aligned} \mathrm{H}_{ijk} &= \left(h_{ipq}h_{jr}h_{ks} + h_{jpq}h_{kr}h_{is} + h_{kpq}h_{ir}h_{js}\right) h_{ab}\eta^{pa}\delta^{qbsr} \\ \delta^{ijkl} &:= \det\begin{pmatrix} \eta^{ik} & \eta^{il} \\ \eta^{jk} & \eta^{jl} \end{pmatrix} \end{aligned} \tag{31}$$

where we use short notations for the derivatives of the Hamiltonian density

$$h_{ij} := \frac{\partial^2 h}{\partial v^i \partial v^j}, \quad h_{ijk} := \frac{\partial^3 h}{\partial v^i \partial v^j \partial v^k}.$$

The tensor (31) is totally antisymmetric. For $n = 1$ and $n = 2$ any hyperbolic system is integrable. For $n \geq 3$ there are $n(n-1)(n-2)/6$ integrability constraints $\mathrm{H}_{ijk} = 0, i < j < k$.

Given a symmetry (29) the functions $v^1(x,t), \ldots, v^n(x,t)$ implicitly defined by the system of n equations written in the form

$$\det\left[(\lambda - x)\cdot \mathrm{id} + t\, A(v) - B(v)\right] \equiv \lambda^n, \quad A(v) = \left(A^i_j(v)\right), \ B(v) = \left(B^i_j(v)\right) \tag{32}$$

give a solution to the original hyperbolic system. Any solution to this system satisfying certain genericity conditions can be obtained in this way [66].

Let us now consider Hamiltonian perturbations

$$u^i_t + \eta^{ij}\partial_x \frac{\delta H}{\delta u^j(x)} = 0, \quad H = H_0 + O(\epsilon), \quad H_0 = \int h(u)\,dx \tag{33}$$

of an integrable hyperbolic system

$$v^i_t + \eta^{ij}\partial_x \frac{\delta H_0}{\delta v^j(x)} = 0, \quad i = 1, \ldots, n. \tag{34}$$

(We use different notations $v = v(x,t)$ and $u = u(x,t)$ for the dependent variables of the unperturbed/perturbed systems resp. for a convenience later on.)

Definition 5. The perturbed system (33) is called N-integrable if there exists a linear differential operator

$$\begin{aligned} &D_N = D^{[0]} + \epsilon D^{[1]} + \epsilon^2 D^{[2]} + \cdots + \epsilon^N D^{[N]} \\ &D^{[0]} = \mathrm{id}, \quad D^{[k]} = \sum b^{[k]}_{i_1,\ldots,i_{m(k)}}(u; u_x, \ldots, u^{(k)}) \frac{\partial^{m(k)}}{\partial u^{i_1} \ldots \partial u^{i_{m(k)}}} \\ &\deg b^{[k]}_{i_1,\ldots,i_{m(k)}}(u; u_x, \ldots, u^{(k)}) = k, \quad k \geq 1 \end{aligned} \tag{35}$$

acting on the commuting Hamiltonians (28)–(30) such that, for any two solutions $f(u)$, $g(u)$ to (28) the Hamiltonians

$$H_N^f := \int D_N f \, dx, \qquad H_N^g := \int D_N g \, dx \tag{36}$$

satisfy

$$\{H_N^f, H_N^g\} = O\left(\epsilon^{N+1}\right). \tag{37}$$

Moreover, we require that

$$H = D_N h + O\left(\epsilon^{N+1}\right), \tag{38}$$

so the Hamiltonians (36) satisfy also

$$\{H, H_N^f\} = O\left(\epsilon^{N+1}\right)$$

for any solution $f = f(u)$ to (28).

The perturbed system (33) is called integrable if it is N-integrable for any $N \geq 0$.

In the formula (35) $m(k)$ is some positive integer depending on k. The summation is taken over all indices $i_1, \ldots, i_{m(k)}$ from 1 to n. As usual the coefficients $b^{[k]}_{i_1 \ldots i_{m(k)}}(u; u_x, \ldots, u^{(k)})$ are graded homogeneous differential polynomials of degree k. It is easy to see that

$$m(k) = \left[\frac{3k}{2}\right]. \tag{39}$$

As the D-operator makes sense only acting on the common kernel of the linear operators

$$h_{jk}\eta^{ij}\frac{\partial^2}{\partial v^i \partial v^l} - h_{jl}\eta^{ij}\frac{\partial^2}{\partial v^i \partial v^k}, \quad k, l = 1, \ldots, n, \tag{40}$$

the coefficients are not determined uniquely.

For a N-integrable system any symmetry (28)–(30) can be extended to a Hamiltonian flow

$$\begin{aligned} &u^i_s + \eta^{ij}\partial_x \frac{\delta F}{\delta u^j(x)} = 0 \\ &F = F_0 + O(\epsilon), \quad F_0 = \int f(u)\, dx, \quad F = \int D_N f \, dx \end{aligned} \tag{41}$$

satisfying

$$\frac{\partial}{\partial s}\frac{\partial u^i}{\partial t} - \frac{\partial}{\partial t}\frac{\partial u^i}{\partial s} = O\left(\epsilon^{N+1}\right), \quad i = 1, \ldots, n. \tag{42}$$

All these symmetries commute pairwise modulo terms of order ϵ^{N+1}.

The linear differential operator D_N giving an extension of the symmetries of the dispersionless system will be called *D-operator* for an N-integrable system. For an

integrable system such an operator exists for any N; in this case we will omit the label N.

Example 6. The D-operator for the KdV hierarchy has the form

$$f \mapsto Df = \frac{1}{\sqrt{2}} \operatorname{res} \left(\partial^{1/2} f \right) (L), \quad L = \frac{\epsilon^2}{2} \partial_x^2 + u(x). \tag{43}$$

Here $f = f(u)$ is an arbitrary function. In particular choosing

$$f(u) = \frac{u^{k+2}}{(k+2)!}$$

one obtains the Hamiltonian densities of the KdV hierarchy

$$Df = \frac{1}{\sqrt{2}} \frac{2^{k+2}}{(2k+3)!!} \operatorname{res} L^{\frac{2k+3}{2}}.$$

Starting from the above definition we develop a "perturbative" approach to the study of integrability that can be used for

- Finding obstructions to integrability;
- Classification of integrable PDEs.

Example 7. One-dimensional system of particles with neighboring interaction

$$H = \sum \frac{1}{2} p_n^2 + P(q_n - q_{n-1}) \tag{44}$$

with the potential $P(u)$ (generalized Fermi - Pasta - Ulam system) after interpolation

$$\begin{aligned} q_n(t) - q_{n-1}(t) &= w(\epsilon n, \epsilon t) \\ p_n(t) &= v(\epsilon n, \epsilon t) \end{aligned} \tag{45}$$

and substitution

$$u = \frac{\epsilon \partial_x}{1 - e^{-\epsilon \partial_x}} w \tag{46}$$

the following system

$$\begin{aligned} u_t &= v_x \\ v_t &= \epsilon^{-1} \left[P' \left(\frac{e^{\epsilon \partial_x} - 1}{\epsilon \partial_x} u \right) - P' \left(\frac{1 - e^{-\epsilon \partial_x}}{\epsilon \partial_x} u \right) \right] \\ &= \partial_x P'(u) + \frac{\epsilon^2}{24} \left[2P''(u) u_{xxx} + 4P'''(u) u_x u_{xx} + P^{IV}(u) u_x^3 \right] + \mathcal{O}(\epsilon^4). \end{aligned} \tag{47}$$

The above formulae are understood as formal power series in ϵ:

$$w = \frac{e^{\epsilon\partial_x} - 1}{\epsilon\partial_x} u = \frac{1}{\epsilon}\int_x^{x+\epsilon} u(s)\,ds = u + \sum_{k\geq 1} \frac{\epsilon^k}{(k+1)!} u^{(k)},$$
$$u = w + \frac{1}{2}\epsilon w' + \sum_{k>1} \frac{B_k}{k!}\epsilon^k w^{(k)}, \tag{48}$$

B_k are the Bernoulli numbers. Equations (47) is a Hamiltonian system

$$\begin{aligned} u_t &= \partial_x \frac{\delta H}{\delta v(x)} \\ v_t &= \partial_x \frac{\delta H}{\delta u(x)} \\ H &= \int h\,dx = \int \left[\frac{1}{2}v^2(x) + P\left(w(x) - w(x-\epsilon)\right)\right] dx \\ h &= \frac{1}{2}v^2 + P(u) - \frac{\epsilon^2}{24}P''(u)u_x^2 + \frac{\epsilon^4}{5760}\left[8P''(u)u_{xx}^2 - P^{IV}(u)u_x^4\right] + \mathcal{O}(\epsilon^6) \end{aligned} \tag{49}$$

(modulo inessential total derivatives).

In the dispersionless limit $\epsilon \to 0$ (47) reduces to the nonlinear wave equation written as a system

$$\begin{aligned} u_t &= v_x \\ v_t &= \partial_x P'(u). \end{aligned} \tag{50}$$

So, the dispersionless system (50) is integrable for an arbitrary potential $P(u)$. The perturbed system (47) is 2-integrable iff the potential $P(u)$ satisfies

$$P''P^{IV} = (P''')^2$$

that is, only for

$$P(u) = ke^{cu} + au + b$$

for some constants a, b, c, k [20]. So, the generalized FPU system (47) is integrable only when it coincides with Toda lattice.

Example 8. The perturbed Riemann wave equation (24) is 5-integrable for an arbitrary choice of the functional parameters $c(u)$, $p(u)$ [19]. Indeed, the first integrals of the unperturbed system have the form

$$F_0 = \int f(v)\,dx$$

for an arbitrary function $f(v)$. Define deformed functionals by the formula

$$F = \int D_{c,p} f\,dx$$

where the D-operator $D_5 \equiv D_{c,p}$ (see [20] for details) transforming the first integrals of the unperturbed system to the first integrals (modulo $O(\epsilon^6)$) of the perturbed one

$$D_{c,p} f = f - \frac{\epsilon^2}{24} c f''' u_x^2 + \epsilon^4 \left[\left(p f''' + \frac{c^2 f^{(4)}}{480} \right) u_{xx}^2 - \left(\frac{c c'' f^{(4)}}{1152} + \frac{c c' f^{(5)}}{1152} + \frac{c^2 f^{(6)}}{3456} + \frac{p' f^{(4)}}{6} + \frac{p f^{(5)}}{6} \right) u_x^4 \right]. \quad (51)$$

It is an interesting open problem to prove existence and uniqueness, for a given pair of the functional parameters $c(u)$, $p(u)$, of an extension to all orders in ϵ of the perturbed system (24) in order to obtain an integrable PDE. So far existence of such an extension is known only for some particular cases including

- KdV: $c(u) = \text{const}$, $p(u) = 0$.
- Volterra lattice
$$\dot{c}_n = c_n(c_{n+1} - c_{n-1}), \quad n \in \mathbb{Z}.$$
Here $c(u) = 2$, $p(u) = -\frac{1}{240}$.
- Camassa–Holm equation (4) has $c(u) = 8u$, $p(u) = \frac{1}{3}u$.

We will now consider a particular class of systems of *bihamiltonian* PDEs. They admit a Hamiltonian description with respect to two Poisson brackets $\{\ ,\ \}_1$ and $\{\ ,\ \}_2$ of the form (8)–(9) with two different Hamiltonians of the form (10):

$$u_t^i = \{u^i(x), H_1\}_1 = \{u^i(x), H_2\}_2, \quad i = 1, \dots, n. \quad (52)$$

The Poisson brackets must satisfy the *compatibility condition*: the linear combination

$$a_1\{\ ,\ \}_1 + a_2\{\ ,\ \}_2$$

must be a Poisson bracket for arbitrary constant coefficients $a_1, a_2 \in \mathbb{R}$. We will now formulate additional assumptions that ensure integrability of the bihamiltonian system (52). Denote $g_1^{ij}(u)$ and $g_2^{ij}(u)$ the contravariant metrics of the form (16) associated with the Poisson brackets $\{\ ,\ \}_1$ and $\{\ ,\ \}_2$ respectively.

Definition 9. We say that the bihamiltonian structure (52) of the form (9) is strongly nondegenerate if none of the roots of the characteristic equation

$$\det\left(g_2^{ij}(u) - \lambda g_1^{ij}(u)\right) = 0 \quad (53)$$

is a locally constant function on $M^n \ni u$. It is called semisimple if these roots are pairwise distinct.

Theorem 10. *Any system of PDEs admitting a bihamiltonian description with respect to a strongly nondegenerate semisimple bihamiltonian structure is integrable.*

Sketch of the proof. Denote $\lambda = w^1(u), \dots, \lambda = w^n(u)$ the roots of the characteristic equation (53). Under assumptions of the theorem these roots give a system of

local coordinates on M^n [27, 29]. In these coordinates any bihamiltonian dispersionless system (34) becomes diagonal. This proves integrability of the dispersionless system.

Let us now construct a complete set of commuting bihamiltonian flows. Without loss of generality we may assume the metric g_1^{ij} to be constant in the coordinates $u^1, \dots, u^n$. For a given $\lambda \in \mathbb{R}$ consider the generalized Miura transformation

$$u^i \mapsto \tilde{u}^i = F^i(u; u_x, \dots; \epsilon; \lambda)$$

reducing the Poisson pencil

$$\{\ ,\ \}_2 - \lambda\{\ ,\ \}_1$$

to the constant form (14):

$$\{\tilde{u}^i(x), \tilde{u}^j(y)\}_2 - \lambda\{\tilde{u}^i(x), \tilde{u}^j(y)\}_1 = -\lambda g_1^{ij}\delta'(x-y).$$

Using triviality of the Poisson cohomology of this bracket (see above) one can prove [25] that the reducing transformation exists for sufficiently large $|\lambda|$. Moreover, it admits an expansion

$$\tilde{u}^i = u^i + \sum_{p\geq 1} \frac{F_p^i(u; u_x, u_{xx}, \dots; \epsilon)}{\lambda^p}, \quad i = 1, \dots, n$$

$$F_p^i(u; u_x, u_{xx}, \dots; \epsilon) = \sum_{k\geq 0} \epsilon^k F_{p,[k]}^i(u; u_x, \dots, u^{(k)}),$$

$$\deg F_{p,[k]}^i(u; u_x, \dots, u^{(k)}) = k.$$

The Hamiltonians

$$H_p^i = \int F_p^i(u; u_x, u_{xx}, \dots; \epsilon)\, dx, \quad i = 1, \dots, n, \quad p = 0, 1, 2, \dots$$

give a complete family of commuting bihamiltonian flows,

$$\{H_p^i, H_q^j\}_{1,2} = 0, \quad i, j = 1, \dots, n,\ p, q = 0, 1, 2, \dots$$

Taking into account the previous theorems, we will now focus on the deformation theory of bihamiltonian PDEs. A compatible pair of Poisson brackets defines a pair of anticommuting differentials

$$\partial_1^2 = \partial_2^2 = \partial_1\partial_2 + \partial_2\partial_1 = 0$$

on the local multivectors on the loop space $\mathcal{L}(M^n)\otimes\mathbb{R}[[\epsilon]]$. Cohomologies of any of these differentials vanish in positive degrees in ϵ (see above). Define *bihamiltonian cohomology* by

$$H^k(\partial_1, \partial_2) = \frac{\mathrm{Ker}\partial_1\partial_2|_{\Lambda^{k-1}}}{(\mathrm{Im}\partial_1 + \mathrm{Im}\partial_2)_{\Lambda^{k-2}}}, \quad k \geq 2.$$

For $k = 1$ the denominator vanishes; for $k = 0$ the bihamiltonian cohomology is defined by

$$H^0(\partial_1, \partial_2) = \mathrm{Ker}\partial_1 \cap \mathrm{Ker}\partial_2.$$

In particular, the second bihamiltonian cohomology describes the infinitesimal deformation space of a given dispersionless bihamiltonian structure.

Let us first make a digression about dispersionless bihamiltonian structures (also called bihamiltonian structures of the hydrodynamic type)

$$\begin{aligned}\{v^i(x), v^j(y)\}_2 - \lambda\{v^i(x), v^j(y)\}_1 \\ = \left(g_2^{ij}(v(x)) - \lambda g_1^{ij}(v(x))\right)\delta'(x-y) \\ + \left(\Gamma_k^{ij}{}_1(v) - \lambda\Gamma_k^{ij}{}_2(v)\right)v_x^k\delta(x-y).\end{aligned} \tag{54}$$

The metrics $g_1^{ij}(v)$ and $g_2^{ij}(v)$ form a so-called *flat pencil* [16], i.e., the contravariant Christoffel coefficients for the metric $g_2^{ij}(v) - \lambda g_1^{ij}(v)$ are equal to

$$\Gamma_k^{ij}{}_1(v) - \lambda\Gamma_k^{ij}{}_2(v)$$

where

$$\Gamma_k^{ij}{}_1(v) = -g_1^{is}(v)\Gamma_{sk1}^j(v) \quad \text{and} \quad \Gamma_k^{ij}{}_2(v) = -g_2^{is}(v)\Gamma_{sk2}^j(v)$$

are the contravariant Christoffel coefficients for the metrics $g_1^{ij}(v)$ and $g_2^{ij}(v)$ resp. Moreover the curvature of the metric $g_2^{ij}(v) - \lambda g_1^{ij}(v)$ must vanish identically in λ. Assuming the bihamiltonian structure (54) to be strongly nondegenerate and semi-simple one can reduce [27, 33, 56] the theory of flat pencils of metrics to the study of compatibility conditions

$$\begin{aligned}&\partial_k\gamma_{ij} = \gamma_{ik}\gamma_{kj}, \quad i, j, k \text{ distinct} \\ &\partial_i\gamma_{ij} + \partial_j\gamma_{ji} + \sum_{k\neq i,j}\gamma_{ki}\gamma_{kj} = 0 \\ &w^i\partial_i\gamma_{ij} + w^j\partial_j\gamma_{ji} + \sum_{k\neq i,j}w^k\gamma_{ki}\gamma_{kj} + \frac{1}{2}(\gamma_{ij} + \gamma_{ji}) = 0\end{aligned}$$

of the following overdetermined system of linear differential equations with rational coefficients for an auxiliary vector function $\psi = (\psi_1(w), \ldots, \psi_n(w))$

$$\begin{aligned}&\partial_i\psi_j = \gamma_{ji}\psi_i, \quad i \neq j \\ &\partial_i\psi_i + \sum_{k\neq i}\gamma_{ki}\frac{w^k - \lambda}{w^i - \lambda}\psi_k + \frac{1}{2(w^i - \lambda)}\psi_i = 0.\end{aligned} \tag{55}$$

Here $w^1, \dots, w^n$ are the roots of the characteristic equation (53); in these coordinates both the metrics become diagonal

$$\frac{\partial w^i}{\partial v^k}\frac{\partial w^j}{\partial v^l} g_1^{kl}(v) = g_1^{ii}(w)\delta^{ij}, \quad \frac{\partial w^i}{\partial v^k}\frac{\partial w^j}{\partial v^l} g_2^{kl}(v) = w^i g_1^{ii}(w)\delta^{ij}.$$

The coefficients $\gamma_{ij} = \gamma_{ij}(w)$ in (55) are the rotation coefficients of the first metric

$$\gamma_{ij}(w) := H_i^{-1}\partial_i H_j, \quad i \neq j, \quad H_i = \left(g_1^{ii}(w)\right)^{-1/2}. \tag{56}$$

To the best of our knowledge all nontrivial examples of flat pencils of metrics come from Frobenius manifolds (see below).

Let us now consider an ϵ-deformation of the Poisson pencil (54)

$$\begin{aligned}
&\{u^i(x), u^j(y)\}_2 - \lambda\{u^i(x), u^j(y)\}_1 \\
&\quad = \left(g_2^{ij}(u(x)) - \lambda g_1^{ij}(u(x))\right)\delta'(x-y) + \left(\Gamma_k^{ij}{}_1(u) - \lambda\Gamma_k^{ij}{}_2(u)\right)u_x^k\delta(x-y) \\
&\qquad + \sum_{k\geq 1}\epsilon^k \sum_{l=0}^{k+1}\Big[A_{k,l;2}^{ij}(u(x); u_x, \dots, u^{(l)}) \\
&\qquad - \lambda A_{k,l;1}^{ij}(u(x); u_x, \dots, u^{(l)})\Big]\delta^{(k-l+1)}(x-y) \\
&\qquad \deg A_{k,l;a}^{ij}(u; u_x, \dots, u^{(l)}) = l, \quad a = 1, 2.
\end{aligned} \tag{57}$$

We begin with formulating an important *quasitriviality theorem* [27] saying that the bihamiltonian cohomology becomes trivial as soon as we extend the class of generalized Miura transformations allowing rational dependence on the jet coordinates.

Definition 11. The bihamiltonian structure (57) is said to be *trivial* if it can be obtained from the leading term (54) by a λ-independent Miura-type transformation

$$\begin{aligned}
u^i &= v^i + \sum_{k\geq 1}\varepsilon^k F_k^i(v; v_x, \dots, v^{(k)}), \\
&\deg F_k^i(v; v_x, \dots, v^{(k)}) = k, \quad i = 1, \dots, n
\end{aligned} \tag{58}$$

where the coefficients $F_k^i(v; v_x, \dots, v^{(k)})$ are graded homogeneous polynomials in the derivatives. It is called *quasitrivial* if it is not trivial and there exists a transformation

$$u^i = v^i + \sum_{k\geq 1}\varepsilon^k F_k^i(v; v_x, \dots, v^{(m_k)}) \tag{59}$$

reducing (57) to (54) but the functions F_k^i depend *rationally* on the jet coordinates $v^{i,m}$, $m \geq 1$ with

$$\deg F_k^i(v; v_x, \dots, v^{(m_k)}) = k, \quad i = 1, \dots, n, \quad k \geq 1 \tag{60}$$

and m_k are some positive integers. If such a transformation (58) or (59) exists, it is called a *reducing transformation* of the bihamiltonian structure (57).

Example 12. For the Poisson pencil known in the theory of KdV hierarchy

$$\{u(x),u(y)\}_2-\lambda\{u(x),u(y)\}_1=(u(x)-\lambda)\,\delta'(x-y)+\frac{1}{2}u_x\delta(x-y)+\frac{1}{8}\epsilon^2\delta'''(x-y) \tag{61}$$

the reducing transformation reads

$$u=v-\frac{\epsilon^2}{12}(\log v_x)_{xx}+\epsilon^4\left[\frac{v_{xxxx}}{288v_x^2}-\frac{7v_{xx}v_{xxx}}{480v_x^3}+\frac{v_{xx}^3}{90v_x^4}\right]_{xx}+O(\epsilon^6). \tag{62}$$

It is a canonical transformation

$$v\mapsto u=v+\epsilon\{v(x),K\}+\frac{\epsilon^2}{2}\{\{v(x),K\},K\}+\cdots$$

generated by the Hamiltonian

$$K=-\int\left[\frac{\epsilon}{24}v_x\log v_x+\frac{\epsilon^3}{5760}\frac{v_{xx}^3}{v_x^3}+O(\epsilon^5)\right]dx. \tag{63}$$

Theorem 13 (See [27][3]). *Any strongly nondegenerate semisimple bihamiltonian structure (57) is quasitrivial. The coefficients F_k^i of the reducing transformation (59) have the form*

$$F_k^i(v;v_x,\dots,v^{(m_k)})\in C^\infty(M^n)\left[v_x,\dots,v^{(m_k)}\right]\left[\left(w_x^1w_x^2\dots w_x^n\right)^{-1}\right]$$
$$m_k\le\left[\frac{3k}{2}\right]. \tag{64}$$

Here $w^i=w^i(v)$ are the roots of the characteristic equation (53).

The reducing transformation for the bihamiltonian structure (57) establishes a correspondence between solutions of any bihamiltonian system (52) admitting regular expansion in ϵ

$$u^i(x,t;\epsilon)=u_0^i(x,t)+\sum_{k\ge1}\epsilon^k u_k^i(x,t),\quad i=1,\dots,n$$

and monotone solutions to the dispersionless limit

$$v_t^i=\{v^i(x),H_1^0\}_1^0=\{v^i(x),H_2^0\}_2^0,\quad i=1,\dots,n$$
$$\{\,,\,\}_{1,2}^0:=\{\,,\,\}_{1,2}|_{\epsilon=0},\qquad H_{1,2}^0:=H_{1,2}|_{\epsilon=0}. \tag{65}$$

[3] For $n=1$ the proof of quasitriviality theorem was also obtained in [1]. Apparently the author of [1] was not aware about results of the paper [27].

By definition the solution $v = v(x,t)$ is called monotone if

$$\partial_x w^i(v(x,t)) \neq 0, \quad i = 1, \dots$$

for all real x, t.

Therefore the problem of solving of any system of bihamiltonian PDEs of the above form can be reduced to solving *linear PDEs* (28) (see details in [27]).

We will now address the problem of classification of bihamiltonian structures (57) with a *given* dispersionless limit (54). First we will associate with any such a perturbation a collection of n functions of one variable called central invariants [51, 27, 29]. With any Poisson bracket of the form (9) we associate a matrix valued series in an auxiliary variable p:

$$\pi^{ij}(u;\, p) = \sum_{k\geq 0} A^{ij}_{k,0}(u) p^k. \tag{66}$$

Recall that the coefficients $A^{ij}_{k,0}$ have degree 0 in the jet variables, so they may depend only on u. In this way for a bihamiltonian structure one obtains two matrix valued series $\pi_1^{ij}(u;\, p)$ and $\pi_2^{ij}(u;\, p)$. Recall that the leading terms of these series are $A^{ij}_{0,0_1}(u) = g_1^{ij}(u)$, $A^{ij}_{0,0_2}(u) = g_2^{ij}(u)$. Consider the characteristic equation

$$\det\left(\pi_2^{ij}(u;\, p) - \lambda \pi_1^{ij}(u;\, p)\right) = 0. \tag{67}$$

The roots $\lambda^i(u;\, p), \dots, \lambda^n(u;\, p)$ have the form

$$\lambda^i(u;\, p) = \sum_{k\geq 0} \lambda^i_k(u) p^k, \quad \lambda^i_0(u) = w^i(u), \quad \lambda^i_k(u) = 0 \quad \text{for } k = \text{odd}.$$

Put

$$c_i = \frac{1}{3} \frac{\lambda^i_2(u)}{g_1^{ii}(w)}, \quad i = 1, \dots, n. \tag{68}$$

Definition 14. The functions $c_i \in \mathcal{C}^\infty(M^n)$ are called *central invariants* of the bihamiltonian structure (57).

Theorem 15 (See [51, 27, 29]).

(1) *The central invariant c_i is a function of one variable w^i, $i = 1, \dots, n$.*
(2) *Two strongly nondegenerate semisimple bihamiltonian structures are equivalent* iff *they have the same central invariants. In particular, the bihamiltonian structure is trivial* iff *it has all central invariants equal zero.*

Example 16. For the bihamiltonian structure (61) the central invariant is constant $c_1 = \frac{1}{24}$. For the bihamiltonian structure of the Camassa–Holm hierarchy

$$\{u(x), u(y)\}_2 - \lambda\{u(x), u(y)\}_1 = (u(x) - \lambda)\,\delta'(x-y) + \frac{1}{2}u_x\delta(x-y) + \lambda\frac{\epsilon^2}{8}\delta'''(x-y)$$

the central invariant equals

$$c_1 = \frac{1}{24}w, \quad w = u.$$

So the KdV and Camassa–Holm hierarchies are not equivalent.

The theory of central invariants gives a description of the space of infinitesimal deformations of bihamiltonian systems of hydrodynamic type. It remains an open problem to prove vanishing of higher obstructions and establish existence of an integrable hierarchy with a given dispersionless limit and given central invariants. In the next section we will formulate some partial existence results for bihamiltonian PDEs associated with semisimple Frobenius manifolds.

4 Frobenius Manifolds and Integrable Hierarchies of the Topological Type

Frobenius structures on M^n yield a particular subclass of bihamiltonian structure of hydrodynamic type on the loop space $\mathcal{L}(M^n)$. Recall [18] that a Frobenius structure $(\cdot, e, \langle\ ,\ \rangle, E, d)$ on M^n consists of a structure of a Frobenius algebra[4] $(x, y) \mapsto x \cdot y \in T_vM^n$ on the tangent spaces $T_vM^n = (A_v, \langle\ ,\ \rangle_v)$ depending (smoothly, analytically etc.) on the point $v \in M^n$. It must satisfy the following axioms.

FM1. The curvature of the metric $\langle\ ,\ \rangle_v$ on M^n vanishes. Denote ∇ the Levi-Civita connection for the metric. The unity vector field e must be flat, $\nabla e = 0$.

FM2. Let c be the 3-tensor $c(x, y, z) := \langle x \cdot y, z\rangle$, $x, y, z \in T_vM^n$. The 4-tensor $(\nabla_w c)(x, y, z)$ must be symmetric in $x, y, z, w \in T_vM^n$.

FM3. A *linear* vector field $E \in Vect(M^n)$ (called *Euler vector field*) must be fixed on M^n, i.e. $\nabla\nabla E = 0$, such that

$$Lie_E(x \cdot y) - Lie_E x \cdot y - x \cdot Lie_E y = x \cdot y$$
$$Lie_E\langle\ ,\ \rangle = (2-d)\langle\ ,\ \rangle$$

for some number $d \in k$ called *charge*.

In the flat coordinates $v^1, \ldots, v^n$ for the metric $\langle\ ,\ \rangle$ the structure constants of the algebra structure are locally given by triple derivatives of a function $F(v)$ called *potential* of the Frobenius manifold:

[4] Recall that a commutative associative unital algebra A over a field k is called *Frobenius algebra* if it is equipped with a nondegenerate symmetric *invariant* k-bilinear form, i.e., $\langle x \cdot y, z\rangle = \langle x, y \cdot z\rangle$ for all $x, y, z \in A$.

$$\left\langle \frac{\partial}{\partial v^i} \cdot \frac{\partial}{\partial v^j}, \frac{\partial}{\partial v^k} \right\rangle = \frac{\partial^3 F(v)}{\partial v^i \partial v^j \partial v^k}. \tag{69}$$

This function must satisfy WDVV associativity equations, including the quasihomogeneity condition

$$EF = (3-d)F + \text{quadratic terms}$$

(see details in [18]).

Using the metric $\langle\,,\,\rangle$ one also obtains an algebra structure on the cotangent planes $T_v^* M^n$. The two contravariant metrics (i.e., bilinear forms on M^n) are defined by the following formulae

$$\begin{aligned} (\omega_1, \omega_2)_1 &= \langle \omega_1, \omega_2 \rangle \\ (\omega_1, \omega_2)_2 &= i_E(\omega_1 \cdot \omega_2). \end{aligned} \tag{70}$$

Remarkably this pair of metrics forms a flat pencil. The commuting Hamiltonians of the associated bihamiltonian dispersionless hierarchy are expressed via the horizontal sections of the so-called deformed flat connection on M^n. Any choice of such a basis of horizontal sections gives a *calibration* of the Frobenius manifold.

One of equations of the integrable hierarchy on $\mathcal{L}(M^n)$ has a particularly simple form resembling the Riemann wave equation

$$\mathbf{v}_t + \mathbf{v} \cdot \mathbf{v}_x = 0, \quad \mathbf{v} = (v^1, \dots, v^n) \in M^n \simeq T_{\mathbf{v}} M^n \tag{71}$$

where we identify points of the manifold with points in the tangent plane using the flat coordinates.

We arrive at the problem of *reconstruction* of the integrable hierarchy with the given dispersionless limit (71). This can be done for the case of *semisimple* Frobenius manifolds. By definition the Frobenius structure is called semisimple if the algebra structure on the tangent planes $T_v M^n$ is semisimple for all[5] $v \in M^n$. The bihamiltonian structure associated with the flat pencil of metrics (70) will be strongly nondegenerate semisimple *iff* the Frobenius manifold is semisimple.

Theorem 17. *For any calibrated semisimple Frobenius manifold structure on M^n there exists a unique integrable hierarchy*

$$\begin{aligned} &\frac{\partial u^i}{\partial t^{j,p}} = \partial_x \sum_{g \geq 0} \epsilon^{2g} K^i_{j,p;g}(u; u_x, \dots, u^{(2g)}), \quad i, j = 1, \dots, n, \ p \geq 0 \\ &\deg K^i_{j,p;g}(u; u_x, \dots, u^{(2g)}) = 2g \end{aligned} \tag{72}$$

with the right hand sides polynomial in jets in every order in ϵ with the dispersionless term

$$\frac{\partial v^i}{\partial t^{j,p}} = \partial_x K^i_{j,p;0}(v) \tag{73}$$

defined as above by the Frobenius manifold and all central invariants equal to $1/24$.

[5] Here we are considering only a small ball in the Frobenius manifold. Globally the Frobenius manifolds under consideration are only generically semisimple.

The clue to the proof of this theorem [26] is in invariance of the equations of the hierarchy with respect to the Virasoro symmetries

$$\tau \mapsto \tau + \alpha L_m \tau + O(\alpha^2), \quad m \geq -1 \tag{74}$$

acting linearly onto the tau-function of the hierarchy. The tau-function

$$\tau = \tau(\mathbf{t}; \epsilon) = \exp \sum_{g \geq 0} \epsilon^{2g-2} \mathcal{F}_g(\mathbf{t}), \tag{75}$$

$\mathbf{t} = (t^{i,p})_{1 \leq i \leq n,\ p \geq 0}$ of any solution[6]

$$u^i(x, \mathbf{t}; \epsilon) = \sum_{g \geq 0} \epsilon^{2g} u^i_g(x, \mathbf{t}) \tag{76}$$

to the hierarchy is defined by the equations

$$u^i(x, \mathbf{t}; \epsilon) = \epsilon^2 \eta^{ij} \frac{\partial^2}{\partial x \partial t^{j,0}} \log \tau(\mathbf{t}; \epsilon), \quad i = 1, \ldots, n. \tag{77}$$

Existence of such a tau-function is the main reason for appearance of Frobenius manifolds in the theory of integrable hierarchies [25, 27, 26]. The Virasoro operators have the form [23]

$$\begin{aligned} L_m &= L_m(\epsilon^{-1}\mathbf{t}, \epsilon \partial/\partial \mathbf{t}) \\ &= \sum \epsilon^2 a_m^{i,p;j,q} \frac{\partial^2}{\partial t^{i,p} \partial t^{j,q}} + \sum b_m{}^{i,p}_{j,q} t^{j,q} \frac{\partial}{\partial t^{i,p}} \\ &\quad + \epsilon^{-2} c^m_{i,p;j,q} t^{i,p} t^{j,q} + d_0 \delta_{m,0} \end{aligned} \tag{78}$$

where constant coefficients $a_m^{i,p;j,q}$, $b_m{}^{i,p}_{j,q}$, $c^m_{i,p;j,q}$ for every $m \geq -1$ and d_0 depend on the Frobenius manifold. The hierarchy (72) is obtained from the known dispersionless limit (73) by a quasitriviality transformation of the form

$$v^i \mapsto u^i = v^i + \eta^{ij} \frac{\partial^2}{\partial x \partial t^{j,0}} \sum_{g \geq 0} \epsilon^{2g} F_g(v; v_x, \ldots, v^{(3g-2)}) \tag{79}$$

where the terms of expansion are rational functions of jet variables of the degree

$$\deg F_g(v; v_x, \ldots, v^{(3g-2)}) = 2g - 2, \quad g \geq 2.$$

These terms are determined from the system of *Virasoro constraints* [25]. For example, for $g = 1$ from this procedure one derives

[6] More general solutions admitting regular expansions in ϵ are obtained from (76) by ϵ-dependent shifts $\mathbf{t} \mapsto \mathbf{t} - \mathbf{t}_0(\epsilon)$.

$$F_1 = \frac{1}{24}\sum_{i=1}^{n} \log w^i_x - \log\left(\tau_I(w) J^{1/24}(w)\right), \quad J(w) = \det\left(\frac{\partial v^i}{\partial w^j}\right). \tag{80}$$

Here $\tau_I(w)$ is the so-called isomonodromy tau-function[7] of the Frobenius manifold. The formula (80) was derived in [23] from the universal identities [37] for the genus 1 Gromov–Witten invariants.

Reducing the system of Virasoro constraints to the so-called *universal loop equation* [25, 18] one proves existence [26] and uniqueness [25] of the solution. Moreover, using Virasoro invariance one proves that the resulting hierarchy (72) is polynomial in jet variables in every order in ϵ.

Remark 18. One can also prove that the conserved quantities of (72) obtained by applying the quasitriviality transformation (79) to the Hamiltonians of the dispersionless hierarchy (73) depend polynomially on the jet variables, in every order in ϵ. It remains to prove that also the coefficients of the resulting bihamiltonian structure depend polynomially on the jet variables.

Definition 19. The integrable hierarchy associated by the above construction with a given calibrated semisimple Frobenius manifold M^n is called *integrable hierarchy of the topological type*.

Let us describe the structure of solutions of an integrable hierarchy of the topological type. The *vacuum solution* $\tau_{\text{vac}}(\mathbf{t};\epsilon)$ is defined by the system of Virasoro constraints

$$L_m \tau_{\text{vac}}(\mathbf{t};\epsilon) = 0, \quad m \geq -1. \tag{81}$$

Any other solution to the hierarchy admitting a regular expansion in ϵ is obtained by an ϵ-dependent shift $\mathbf{t} \mapsto \mathbf{t} - \mathbf{t}_0(\epsilon)$. In particular, the *topological solution* is specified by the so-called *dilaton shift*

$$\tau_{\text{top}}(\mathbf{t};\epsilon) = \tau_{\text{vac}}(\mathbf{t} - \mathbf{t}_{\text{dilaton}};\epsilon), \qquad t^{i,p}_{\text{dilaton}} = \delta^i_1 \delta^p_1. \tag{82}$$

The corresponding topological solution (77) to the integrable hierarchy of the topological type admits an expansion

$$u^i_{\text{top}}(x,\mathbf{t};\epsilon) = \sum_{g\geq 0} \epsilon^{2g} \sum_{m\geq 0} \sum_{\mathbf{j},\mathbf{p}} a^i_{\mathbf{j},\mathbf{p},g}(t^{1,0}+x, t^{2,0}, \dots, t^{n,0}) t^{j_1,p_1} \dots t^{j_m,p_m}. \tag{83}$$

Here the summation over multiindices $\mathbf{j}, \mathbf{p} = (j_1, \dots, j_m, p_1, \dots, p_m)$ extends over all values

$$1 \leq j_1, \dots, j_m \leq n, \qquad 1 \leq p_1, \dots, p_m.$$

The coefficients of the expansion are given in terms of certain functions $a^i_{\mathbf{j},\mathbf{p},g}(v^1, \dots, v^n)$ smooth on the semisimple part of the Frobenius manifold. Note that for a generic semisimple Frobenius manifold these functions have a complicated singularity at the origin $v^1 = \dots = v^n = 0$.

[7] We have changed the sign in the definition [23] of the isomonodromy tau-function.

Example 20. For $n = 1$ one has only one Frobenius manifold with the potential $F(v) = \frac{1}{6}v^3$. The associated integrable hierarchy of the topological type coincides with the KdV hierarchy

$$\begin{aligned} u_{t_0} &= u_x \\ u_{t_1} &= uu_x + \frac{\epsilon^2}{12}u_{xxx} \\ u_{t_2} &= \frac{1}{2}u^2u_x + \frac{\epsilon^2}{12}(2u_xu_{xx} + uu_{xxx}) + \frac{\epsilon^4}{240}u^V, \ \dots \end{aligned}$$

represented in the Lax form as follows:

$$\epsilon\frac{\partial L}{\partial t_k} = [A_k, L], \quad L = \frac{\epsilon^2}{2}\frac{d^2}{dx^2} + u, \ A_k = \frac{2^{\frac{2k+1}{2}}}{(2k+1)!!}\left(L^{\frac{2k+1}{2}}\right)_+.$$

The vacuum solution to the KdV hierarchy reads

$$\begin{aligned} \tau^{\text{vac}}_{\text{KdV}} = \frac{1}{(-t_1)^{1/24}}\exp\Bigg\{\frac{1}{\epsilon^2}\Bigg[&-\frac{t_0^3}{6t_1} - \frac{t_0^4t_2}{24t_1^3} + O(t_0^5)\Bigg] \\ &+ \left[\frac{t_0t_2}{24t_1^2} - \frac{t_0^2t_3}{48t_1^3} + \frac{t_0^2t_2^2}{24t_1^4} + O(t_0^3)\right] \\ &+ \epsilon^2\left[-\frac{t_4}{1152t_1^3} + \frac{29t_2t_3}{5760t_1^4} - \frac{7t_2^3}{1440t_1^5} + O(t_0)\right] + O(\epsilon^4)\Bigg\}. \end{aligned} \tag{84}$$

After the dilaton shift $t_1 \mapsto t_1 - 1$ one obtains [68, 47] the generating function of the intersection numbers of the tautological classes $\psi_i = c_1(\mathcal{L}_i) \in H^2(\bar{\mathcal{M}}_{g,n})$ on the moduli spaces $\bar{\mathcal{M}}_{g,n}$ of stable algebraic curves

$$\begin{aligned} \log\tau^{\text{KdV}}_{\text{top}} = \frac{1}{\epsilon^2}\Bigg(&\frac{t_0^3}{6} + \frac{t_0^3t_1}{6} + \frac{t_0^3t_1^2}{6} + \frac{t_0^3t_1^3}{6} + \frac{t_0^3t_1^4}{6} + \frac{t_0^4t_2}{24} + \frac{t_0^4t_1t_2}{8} \\ &+ \frac{t_0^4t_1^2t_2}{4} + \frac{t_0^5t_2^2}{40} + \frac{t_0^5t_3}{120} + \frac{t_0^5t_1t_3}{30} + \frac{t_0^6t_4}{720} + \cdots\Bigg) \\ &+ \Bigg(\frac{t_1}{24} + \frac{t_1^2}{48} + \frac{t_1^3}{72} + \frac{t_1^4}{96} + \frac{t_0t_2}{24} + \frac{t_0t_1t_2}{12} + \frac{t_0t_1^2t_2}{8} + \frac{t_0^2t_2^2}{24} \\ &+ \frac{t_0^2t_3}{48} + \frac{t_0^2t_1t_3}{16} + \frac{t_0^3t_4}{144} + \cdots\Bigg) \\ &+ \epsilon^2\left(\frac{7t_2^3}{1440} + \frac{7t_1t_2^3}{288} + \frac{29t_2t_3}{5760} + \frac{29t_1t_2t_3}{1440} + \frac{29t_1^2t_2t_3}{576} + \frac{5t_0t_2^2t_3}{144}\right. \end{aligned}$$

$$+\frac{29t_0t_3^2}{5760}+\frac{29t_0t_1t_3^2}{1152}+\frac{t_4}{1152}+\frac{t_1t_4}{384}+\frac{t_1^2t_4}{192}+\frac{t_1^3t_4}{96}+\frac{11t_0t_2t_4}{1440}$$
$$+\frac{11t_0t_1t_2t_4}{288}+\frac{17t_0^2t_3t_4}{1920}+\cdots\Bigg)+O(\epsilon^4)$$
$$=\sum_{g\geq 0}\epsilon^{2g-2}\mathcal{F}_g(\mathbf{t}),\quad \mathcal{F}_g(\mathbf{t})=\sum\frac{1}{n!}t_{p_1}\dots t_{p_n}\int_{\bar{\mathcal{M}}_{g,n}}\psi_1^{p_1}\wedge\cdots\wedge\psi_n^{p_n}.$$

The definition (77) of tau-function reduces to a familiar formula

$$u=\epsilon^2\partial_x^2\log\tau,\quad x=t_0$$

for solutions to the KdV hierarchy.

The topological solution $u(x,\mathbf{t})$ can be also characterized by the initial data

$$u(x,0;\epsilon^2)=x.$$

The Virasoro symmetries of the KdV hierarchy are generated by the operators

$$L_m=\frac{\epsilon^2}{2}\sum_{k+l=m-1}\frac{(2k+1)!!(2l+1)}{2^{m+1}}\frac{\partial^2}{\partial t_k\partial t_l}$$
$$+\sum_{k\geq 0}\frac{(2k+2m+1)!!}{2^{m+1}(2k-1)!!}t_k\frac{\partial}{\partial t_{k+m}}+\frac{1}{16}\delta_{m,0},\quad m\geq 0, \tag{85}$$
$$L_{-1}=\sum_{k\geq 1}t^k\frac{\partial}{\partial t_{k-1}}+\frac{1}{2\epsilon^2}t_0^2.$$

Example 21. Choosing the shift vector in the form

$$t_k^0=\frac{(-1)^{k+1}}{k!(k-1)!},\quad k\geq 1,\quad t_0=0$$

one obtains the generating function of the Weil–Petersson volumes of the moduli spaces

$$\log\tau_{\text{top}}^{\text{KdV}}\left(x,-1,\frac{1}{1!2!},-\frac{1}{2!3!},\dots;\epsilon^2\right)$$
$$=\sum_{g=0}^{\infty}\left(\frac{\epsilon}{\pi^3}\right)^{2g-2}\sum_n\text{Vol}(\mathcal{M}_{g,n})\left(\frac{x}{\pi^2}\right)^n. \tag{86}$$

This is a reformulation of the result of P. Zograf and Yu.I. Manin [73, 52].

Example 22. The hierarchy of the topological type associated with the two-dimensional Frobenius manifold with the potential

$$F(u,v)=\frac{1}{2}uv^2+e^u$$

coincides with the *extended Toda hierarchy* [8] associated with the difference Lax operator

$$L = \Lambda + v + e^u \Lambda^{-1}, \quad \Lambda = e^{\epsilon \partial_x}.$$

The hierarchy contains two infinite sequences of time variables

$$\epsilon \frac{\partial L}{\partial t_k} = \frac{1}{(k+1)!}\left[(L^{k+1})_+, L\right], \qquad \epsilon \frac{\partial L}{\partial s_k} = \frac{2}{k!}\left[\left(L^k(\log L - c_k)\right)_+, L\right]$$
$$c_k = 1 + \frac{1}{2} + \cdots + \frac{1}{k}$$

In particular, for $k = 0$ one obtains the standard *Toda lattice equations* (2) written in the form (3), $t = t_0$. The tau-function of a solution $u = u(\mathbf{s}, \mathbf{t}; \epsilon)$, $v = v(\mathbf{s}, \mathbf{t}; \epsilon)$ to the hierarchy is defined by

$$u = \log \frac{\tau(s_0 + \epsilon)\tau(s_0 - \epsilon)}{\tau^2(s_0)}$$
$$v = \epsilon \frac{\partial}{\partial t_0} \log \frac{\tau(s_0 + \epsilon)}{\tau(s_0)}$$

$x = s_0$ (see details in [8]). The Virasoro symmetries of the hierarchy are generated by the operators [24]

$$\begin{aligned} L_m &= \epsilon^2 \sum_{k=1}^{m-1} k!(m-k)! \frac{\partial^2}{\partial t_{k-1} \partial t_{m-k-1}} \\ &\quad + \sum_{k \geq 1} \frac{(m+k)!}{(k-1)!} \left(s_k \partial s_{m+k} + t_{k-1} \frac{\partial}{\partial t_{m+k-1}} \right) \\ &\quad + 2 \sum_{k \geq 0} \alpha_m(k) s_k \frac{\partial}{\partial t_{m+k-1}}, \quad m > 0, \\ L_0 &= \sum_{k \geq 1} k \left(s_k \frac{\partial}{\partial s_k} + t_{k-1} \frac{\partial}{\partial s_{k-1}} \right) + \sum_{k \geq 1} 2 s_k \frac{\partial}{\partial t_{k-1}} + \frac{1}{\epsilon^2} s_0^2, \\ L_{-1} &= \sum_{k \geq 1} \left(t_k \frac{\partial}{\partial t_{k-1}} + s_k \frac{\partial}{\partial s_{k-1}} \right) + \frac{1}{\epsilon^2} s_0 t_0, \end{aligned}$$

$$\alpha_m(0) = m!, \qquad \alpha_m(k) = \frac{(m+k)!}{(k-1)!} \sum_{j=k}^{m+k} \frac{1}{j}, \quad k > 0.$$

According to [38, 59, 24] for the topological solution to the extended Toda hierarchy the tau-functions generates the Gromov–Witten invariants of $\mathbf{P}^1$ and their descendents

$$\log \tau_{\text{top}}(s_0, t_0, s_1, t_1, \ldots; \epsilon^2) = \log \tau_{\text{vac}}(s_0, t_0, s_1 - 1, t_1, \ldots; \epsilon^2) = \sum_{g \geq 0} \epsilon^{2g-2} \mathcal{F}_g$$

$$\mathcal{F}_g = \sum \frac{1}{n!} t_{\alpha_1, p_1} \ldots t_{\alpha_n, p_n} \int_{[\bar{\mathcal{M}}_{g,n}(\mathbf{P}^1, \beta)]} \text{ev}_1^* \phi_{\alpha_1} \wedge \psi_1^{p_1} \wedge \cdots \wedge \text{ev}_n^* \phi_{\alpha_n} \wedge \psi_n^{p_n}.$$

Here $\phi_1 \in H^0(\mathbf{P}^1)$, $\phi_2 \in H^2(\mathbf{P}^1)$ is a basis in the cohomology,

$$t_{1,p} = s_p, \qquad t_{2,p} = t_p,$$
$$\mathcal{M}_{g,n}(\mathbf{P}^1, \beta) = \left\{ f : (C_g, x_1, \dots, x_n) \to \mathbf{P}^1, \ \beta = \text{degree of the map } f \right\}$$

are the moduli spaces of stable maps with values in the complex projective line.

Example 23. Toda hierarchy and enumeration of ribbon graphs/triangulations of Riemann surfaces. A different choice of a shift[8] in the vacuum tau-function of the extended Toda hierarchy gives

$$\log \tau_{\text{vac}}^{\text{Toda}}(s_0, t_0, s_1, t_1 - 1, s_2, t_2, \dots; \epsilon)|_{t_0=t_1=0, t_k=(k+1)!\lambda_{k+1}; s_0=x, \ s_k=0}$$
$$= \frac{x^2}{2\epsilon^2}\left(\log x - \frac{3}{2}\right) + \frac{x}{2\epsilon}\log 2\pi - \frac{1}{12}\log x + \zeta'(-1)$$
$$+ \sum_{g\geq 2}\left(\frac{\epsilon}{x}\right)^{2g-2}\frac{B_{2g}}{2g(2g-2)} + \sum_{g\geq 0}\epsilon^{2g-2}F_g(x; \lambda_3, \lambda_4, \dots)$$

where B_{2g} are Bernoulli numbers, $\zeta(s)$ the Riemann zeta-function,

$$F_g(x; \lambda_3, \lambda_4, \dots) = \sum_n \sum_{k_1,\dots,k_n} a_g(k_1, \dots, k_n)\lambda_{k_1}\dots\lambda_{k_n}x^h,$$
$$h = 2 - 2g - \left(n - \frac{|k|}{2}\right), \quad |k| = k_1 + \dots + k_n,$$

generate the numbers of fat graphs

$$a_g(k_1, \dots, k_n) = \sum_{\Gamma} \frac{1}{\#\text{Sym}\Gamma}$$

where

$$\Gamma = \text{a connected fat graph of genus } g \text{ with } n \text{ vertices of the valencies } k_1, \dots, k_n,$$

Sym Γ is the symmetry group of the graph. E.g., for genus 1, one vertex of valency 4 the unique graph is shown on Fig. 1 (borrowed from [3])

So,

[8] One can show that the new shift corresponds to the topological tau-function of the extended nonlinear Schrödinger hierarchy [24]. The tau-function of the latter is obtained from the tau-function of the extended Toda hierarchy by a permutation of times $t_p \leftrightarrow s_p$, $p \geq 0$.

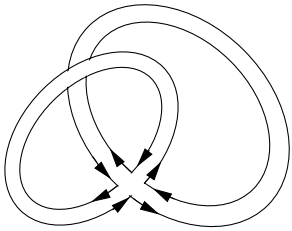

Fig. 1 Fat graph of genus 1 with one vertex of valency 4

$$
\begin{aligned}
F = \epsilon^{-2}\Big[&\frac{1}{2}x^2\Big(\log x - \frac{3}{2}\Big) + 6x^3{\lambda_3}^2 + 2x^3\lambda_4 + 216x^4{\lambda_3}^2\lambda_4 + 18x^4{\lambda_4}^2 \\
&+ 288x^5{\lambda_4}^3 + 45x^4\lambda_3\lambda_5 + 2160x^5\lambda_3\lambda_4\lambda_5 + 90x^5{\lambda_5}^2 + 5400x^6\lambda_4{\lambda_5}^2 \\
&+ 5x^4\lambda_6 + 1080x^5{\lambda_3}^2\lambda_6 + 144x^5\lambda_4\lambda_6 + 4320x^6{\lambda_4}^2\lambda_6 + 10800x^6\lambda_3\lambda_5\lambda_6 \\
&+ 27000x^7{\lambda_5}^2\lambda_6 + 300x^6{\lambda_6}^2 + 21600x^7\lambda_4{\lambda_6}^2 + 36000x^8{\lambda_6}^3\Big] \\
&+ \frac{x}{2\epsilon}\log 2\pi - \frac{1}{12}\zeta'(-1) - \frac{1}{12}\log x + \frac{3}{2}x{\lambda_3}^2 + x\lambda_4 + 234x^2{\lambda_3}^2\lambda_4 \\
&+ 30x^2{\lambda_4}^2 + 1056x^3{\lambda_4}^3 + 60x^2\lambda_3\lambda_5 + 6480x^3\lambda_3\lambda_4\lambda_5 + 300x^3{\lambda_5}^2 \\
&+ 32400x^4\lambda_4{\lambda_5}^2 + 10x^2\lambda_6 + 3330x^3{\lambda_3}^2\lambda_6 + 600x^3\lambda_4\lambda_6 + 31680x^4{\lambda_4}^2\lambda_6 \\
&+ 66600x^4\lambda_3\lambda_5\lambda_6 + 283500x^5{\lambda_5}^2\lambda_6 + 2400x^4{\lambda_6}^2 + 270000x^5\lambda_4{\lambda_6}^2 \\
&+ 696000x^6{\lambda_6}^3 + \epsilon^2\Big[-\frac{1}{240x^2} + 240x{\lambda_4}^3 + 1440x\lambda_3\lambda_4\lambda_5 + \frac{1}{2}165x{\lambda_5}^2 \\
&+ 28350x^2\lambda_4{\lambda_5}^2 + 675x{\lambda_3}^2\lambda_6 + 156x\lambda_4\lambda_6 + 28080x^2{\lambda_4}^2\lambda_6 \\
&+ 56160x^2\lambda_3\lambda_5\lambda_6 + 580950x^3{\lambda_5}^2\lambda_6 + 2385x^2{\lambda_6}^2 + 580680x^3\lambda_4{\lambda_6}^2 \\
&+ 2881800x^4{\lambda_6}^3\Big] + \cdots .
\end{aligned}
$$

The proof uses Toda equations [35, 36] for the Hermitean matrix integral [3, 53]

$$
\begin{aligned}
Z_N(\lambda;\epsilon) =& \frac{1}{\mathrm{Vol}(U_N)}\int_{N\times N} e^{-\frac{1}{\epsilon}\mathrm{Tr}V(A)}\,dA \\
=& \tau_{\mathrm{vac}}^{\mathrm{Toda}}(s_0, t_0, s_1, t_1 - 1, s_2, t_2, \ldots;\epsilon)|_{t_0=t_1=0, t_k=(k+1)!\lambda_{k+1}; s_0=x,\ s_k=0} \\
V(A) =& \frac{1}{2}A^2 - \sum_{k\geq 3}\lambda_k A^k
\end{aligned}
\tag{87}
$$

understood as a formal saddle point expansion near the Gaussian point $\lambda_3 = \lambda_4 = \cdots = 0$ where one has to replace [45]

$$N \mapsto \frac{x}{\epsilon}$$

expanding the normalizing factor

$$\mathrm{Vol}(N) = \frac{2^{N/2}\pi^{\frac{N^2}{2}}\epsilon^{-\frac{N^2}{2}+\frac{1}{12}}}{\prod_{k=0}^{N-1} k!}$$

(related to the volume of the quotient of the unitary group $U(N)$ over the maximal torus $[U(1)]^N$) in the asymptotic series with the help of the asymptotic expansion of Barnes G-function [2]. Observe that the solution $u = u(x, \mathbf{t}, \mathbf{s}; \epsilon)$, $v = v(x, \mathbf{t}, \mathbf{s}; \epsilon)$ associated with the tau-function (87) can be characterized by the initial data

$$e^{u(x,0,0;\epsilon)} = x, \qquad v(x, 0, 0; \epsilon) = 0$$

in agreement with the three term recursion relation

$$2zH_n(z) = H_{n+1}(z) + 2nH_{n-1}(z)$$

for Hermite polynomials. For a convergent matrix integral the formal expansion (87) coincides with the asymptotic expansion of the integral in the so-called one-cut case, i.e., under the assumption that the large N distribution of the eigenvalues of the Hermitean rando matrix A consists of a single interval [30, 31, 4]. The phase transitions from the one-cut to multi-cut behavior can be considered in the general setting of Universality Conjectures of the theory of Hamiltonian PDEs (see below).

Example 24. The Drinfeld–Sokolov construction [14] associates a hierarchy of bihamiltonian integrable systems of the form (8)–(10), (13), (52) with every untwisted Lie algebra $\hat{\mathfrak{g}}$. The associated Frobenius manifold is isomorphic [29] to the one obtained in [15] (for the more general case of orbit spaces of a finite Coxeter group) as the natural polynomial Frobenius structure on the orbit space

$$M^n = \mathfrak{h}/W(\mathfrak{g})$$

of the Weyl group. Here n is the rank of the simple Lie algebra $\mathfrak{g}$, $\mathfrak{h} \subset \mathfrak{g}$ is the Cartan subalgebra. The suitably ordered central invariants of the Drinfeld–Sokolov bihamiltonian structure for an untwisted affine Lie algebra $\hat{\mathfrak{g}}$ are given by the formula [29]

$$c_i = \frac{1}{48}\langle \alpha_i^\vee, \alpha_i^\vee \rangle_{\mathfrak{g}}, \quad i = 1, \dots, n, \tag{88}$$

where $\alpha_i^\vee \in \mathfrak{h}$ are the coroots of the simple Lie algebra $\mathfrak{g}$. Here $\langle\ ,\ \rangle_{\mathfrak{g}}$ is the normalized Killing form,

$$\langle a, b\rangle_{\mathfrak{g}} := \frac{1}{2h^\vee}\,\mathrm{tr}(\mathrm{ad}\, a \cdot \mathrm{ad}\, b), \tag{89}$$

where $h^\vee$ is the dual Coxeter number. Thus, the Drinfeld–Sokolov hierarchy is equivalent to an integrable hierarchy of the topological type only for simply laced simple Lie algebras $\mathfrak{g}$.

We will not discuss here other examples of integrable hierarchies of the topological type. For convenience of the reader we give a list of some important examples[9] of Frobenius manifolds and the associated known, but not only, integrable hierarchies of the topological type.[10] Some of the applications to Gromov–Witten invariants and oscillatory asymptotics mentioned in this table still exist only as conjectures.

Recall that the potential of a generic semisimple Frobenius manifold of dimension $n \geq 3$ is expressed via solutions of certain monodromy preserving deformation equations (for $n = 3$ reducing to Painlevé-VI transcendents). So, the coefficients of a generic integrable hierarchy of the topological type will be expressed via these transcendents. The hierarchies shown in Table 1 correspond to particular solutions to the monodromy preserving deformation equations reducing to classical special functions.

Table 1 List of some Frobenius manifolds and the associated integrable hierarchies of the topological type

$n = 1$	$F = \frac{1}{6}v^3$	KdV
$n = 2$	$F = \frac{1}{2}uv^2 + u^4$	Boussinesq
$n = 2$	$F = \frac{1}{2}uv^2 + e^u$	Toda
$n = 2$	$F = \frac{1}{2}uv^2 + \frac{1}{2}u^2(\log u - \frac{3}{2})$	NLS
$n = 2$	$F = \frac{1}{2}uv^2 - Li_3(e^{-u})$	Ablowitz–Ladik
$n = 3$	$F = \frac{1}{2}(uw^2 + u^2v) + \frac{1}{6}v^2w^2 + \frac{1}{60}w^5$	Drinfeld–Sokolov hierarchy of A_3 type, intersection theory on the moduli spaces of "spin 3 curves" [70, 32]
$n = 3$	$F = \frac{1}{2}(uv^2 + vw^2) - \frac{1}{24}w^4 + 4we^u$	A generalization of Toda hierarchy [7] for a difference Lax operator of bidegree (2,1); orbifold Gromov–Witten invariants of an orbicurve with one point of order 2 [55]
$n = 3$	$F = \frac{1}{2}(\tau v^2 + vu^2) - \frac{i\pi}{48}u^4E_2(\tau)$	Higher corrections to elliptic Whitham asymptotics, the KdV case
$n = 4$	$F = \frac{i}{4\pi}\tau v^2 - 2uvw + u^2\log[\frac{\pi}{u}\frac{\theta_1'(0\|\tau)}{\theta_1(2w\|\tau)}]$	Higher corrections to elliptic Whitham asymptotics, the Toda/NLS case

Remark 25. Very recently the theory of Gromov–Witten invariants of orbicurves with polynomial quantum cohomology has been addressed by P. Rossi [61]. (Previously the theory of Gromov–Witten invariants of the same orbicurves has been analyzed by A. Takahashi from the point of view of homological mirror symmetry

[9] We do not consider here an interesting example of the hierarchy, obtained by a nonstandard reduction [40] of the 2D Toda involved in the description of the equivariant GW invariants [60] of $\mathbf{P}^1$. It remains to better understand the place of this hierarchy in our general framework.

[10] Strictly speaking the example of Ablowitz–Ladik hierarchy does not fit into the general scheme as the function F does not satisfy the quasihomogeneity condition. Nevertheless, the Ablowitz–Ladik hierarchy possesses many properties of integrable hierarchies of the topological type. We will consider this example in a separate publication.

[63].) Rossi proved that for all these orbicurves[11] the associated Frobenius manifold coincides with the one defined by Y. Zhang and the author in [22] on the orbit spaces of simply laced extended affine Weyl groups. It would be interesting to obtain a realization of the associated integrable hierarchies of the topological type and relate it with the higher genus orbifold Gromov–Witten invariants and their descendents.

At the end of this section we will explain a connection [26] of the theory of integrable hierarchies of the topological type with A. Givental's theory of the so-called total descendent potential [41] associated with an arbitrary semisimple Frobenius manifold.

Let H be a n-dimensional linear space equipped with a symmetric nondegenerate bilinear form $\langle\ ,\ \rangle$. Denote $\mathcal{H}$ the *Givental symplectic space* of the H-valued functions on the unit circle $|z| = 1$ that can be extended to an analytic function in an annulus. A symplectic structure on $\mathcal{H}$ is defined by the formula

$$\omega(f, g) := \frac{1}{2\pi i} \oint_{|z|=1} \langle f(-z), g(z)\rangle dz. \tag{90}$$

A natural polarization

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_- \tag{91}$$

is given by the subspaces $\mathcal{H}_+/\mathcal{H}_-$ of functions that can be continued analytically inside/outside the unit circle (the functions in $\mathcal{H}_-$ must also vanish at $z = \infty$). Explicitly the canonical coordinates are given by the components $q^{\alpha,k}$, $p_{\alpha,k}$ of the coefficients of the Laurent expansion

$$f(z) = \cdots - p_2^* z^2 + p_1^* z - p_0^* + \frac{q^0}{z} + \frac{q^1}{z^2} + \cdots . \tag{92}$$

Here we consider $q^k \in H$, $p_k \in H^*$,

$$q^k = q^{\alpha,k} e_\alpha, \qquad p_k = p_{\alpha,k} e^\alpha, \tag{93}$$

$e_1, \ldots, e_n$ is a basis in H, $e^1, \ldots, e^n$ is the dual basis in H^*.

Any matrix valued function $G(z)$ on the unit circle $|z| = 1$ with values in $Aut(H)$ satisfying

$$G^*(-z)G(z) = 1 \tag{94}$$

defines a symplectomorphism

$$G : \mathcal{H} \to \mathcal{H}, \qquad f(z) \mapsto G(z) f(z), \qquad \omega(Gf, Gg) = \omega(f, g). \tag{95}$$

Quantising the symplectomorphism (95) one obtains a *quantum canonical transformation* $\hat{G}$ acting on the Fock space $S^\bullet \mathcal{H}_-$ of functionals on the space $\mathcal{H}_-$ of vector-valued functions

[11] The class of orbicurves considered in [61] includes the orbicurves with two singularities. For this subclass the relationship with the extended affine Weyl groups of A type has been established by T. Milanov and H.-H. Tseng [55].

$$q(z) = \frac{q_0}{z} + \frac{q_1}{z^2} + \cdots, \quad q_k \in H, \ |z| > 1 \tag{96}$$

analytic on the exterior part of the unit circle. The Fock space can be realized by polynomials in an infinite sequence of variables $t^{i,k}$, $i = 1, \ldots, n$, $k \geq 0$. The operators $\hat{q}^{i,k}$ act on the Fock space by multiplication by $\epsilon^{-1} t^{i,k}$ and the operators $\hat{p}_{i,k}$ act by differentiation

$$\hat{q}^{i,k} f(\mathbf{t}) = \epsilon^{-1} t^{i,k} f(\mathbf{t}), \quad \hat{p}_{i,k} = \epsilon \frac{\partial}{\partial t^{i,k}} f(\mathbf{t}). \tag{97}$$

The quantization of $\hat{G}$ can be easily achieved in case the logarithm $g(z) = \log G(z)$ is well defined. Indeed, let us consider the quadratic Hamiltonian

$$H_g = \frac{1}{4\pi i} \oint_{|z|=1} \langle f(-z), g(z) f(z) \rangle dz = \frac{1}{2} p A p^* + q^* B p^* + \frac{1}{2} q^* C q \tag{98}$$

for some semiinfinite matrices A, B, C. The symplectomorphism G is the time 1 shift generated by the Hamiltonian H_g. Put

$$\hat{G} := e^{\hat{H}_g} \tag{99}$$

where

$$\hat{H}_g =: H_g(\hat{p}, \hat{q}) := \frac{1}{2} \epsilon^2 \frac{\partial}{\partial t} A \left(\frac{\partial}{\partial t} \right)^* + t^* B \left(\frac{\partial}{\partial t} \right)^* + \frac{1}{2\epsilon^2} t^* C t \tag{100}$$

is the standard normal ordering quantization of the quadratic Hamiltonian.

A more general situation occurs when the function $G(z)$ admits a Riemann–Hilbert factorization

$$G(z) = G_0^{-1}(z) G_\infty(z), \quad |z| = 1 \tag{101}$$

where the matrix valued functions $G_0(z)$ and $G_\infty(z)$ are analytic and invertible for $|z| < 1$ and $1 < |z| \leq \infty$ resp. The solution, if exists, is uniquely determined by the normalization condition $G_\infty(\infty) = 1$. The logarithms $g_0(z) = \log G_0(z)$ and $g_\infty(z) = \log G_\infty(z)$ are obviously well defined. Therefore one obtains the quantized operators $\hat{G}_0$ and $\hat{G}_\infty$ by applying the formula (99). Put

$$\hat{G} := \gamma_G \hat{G}_0^{-1} \hat{G}_\infty \tag{102}$$

for a suitable multiplier γ_G.

The Givental's formula expresses the so-called total descendent potential as the result of action of a suitable quantum canonical transformation onto a particular element of the (completed) Fock space. The latter is chosen in the form of a product of n copies of vacuum tau-functions (84) of the KdV hierarchy

$$\tau_{\mathrm{KdV}}^{vac}(\mathbf{t}^1; \epsilon^2) \ldots \tau_{\mathrm{KdV}}^{vac}(\mathbf{t}^n; \epsilon^2). \tag{103}$$

Here

$$\mathbf{t}^i = (t^{i,0}, t^{i,1}, t^{i,2}, \dots), \quad i = 1, \dots, n.$$

The last step of the Givental's construction is in the choice of the symplectomorphism $G(z)$. At this point one has to use the parametrization of semisimple Frobenius manifolds by the data of certain Riemann–Hilbert problem [17, 18]. Reducing the Riemann–Hilbert problem to the standard form (101) one obtains a matrix valued function $G_w(z)$ on the unit circle satisfying (94) depending on the point $w \in M^n$ of the Frobenius manifold, and also depending on $n(n-1)/2$ *monodromy data* (the moduli of semisimple Frobenius manifolds; see details in [18]). Givental proves that the result of action of the quantized canonical transformation $\hat{G}_w$ on the vector (103) is well defined in every order in ϵ. Moreover, he proves that the function

$$\hat{G}_w \tau^{vac}_{\mathrm{KdV}}(\mathbf{t}^1; \epsilon^2) \dots \tau^{vac}_{\mathrm{KdV}}(\mathbf{t}^n; \epsilon^2) \tag{104}$$

does not depend on the choice of the semisimple point w when choosing

$$\gamma_G = \tau_I^{-1}(w)$$

the multiplier in the quantization formula (102).

Theorem 26. *For an arbitrary semisimple Frobenius manifold the function* (104) *is the vacuum tau-function for the integrable hierarchy of the topological type associated with the Frobenius manifold. The Givental's total descendent potential is the tau-function of the topological solution to the hierarchy obtained by the dilaton shift* (82)

Proof is based on the representation of the Givental's formula in the form

$$\begin{aligned}\hat{G}_w \tau^{vac}_{\mathrm{KdV}}(\mathbf{t}^1; \epsilon^2) \dots \tau^{vac}_{\mathrm{KdV}}(\mathbf{t}^n; \epsilon^2) \\ = \exp\left[\frac{1}{\epsilon^2}\mathcal{F}_0 + \sum_{g\geq 1} \epsilon^{2g-2} F_g(v; v_x, \dots, v^{(3g-2)})\right]\end{aligned}$$

where

$$v^i = \eta^{ij} \frac{\partial^2 \mathcal{F}_0}{\partial x \partial t^{j,0}}$$

and using validity of the Virasoro constraints for this function proven in [41]. The theorem then follows from the uniqueness of the solution to the system of Virasoro constraints [25].

Corollary 27. *Consider the semisimple Frobenius manifold* $M^n_{\mathbf{P}^N} = QH^*(\mathbf{P}^N)$, $n = N+1$, *given by the quantum cohomology of the* N*-dimensional complex projective space. Then the total Gromov–Witten potential* $\mathcal{F}^{\mathbf{P}^N}(\mathbf{t}; \epsilon^2)$ (*see the formula* (105) *below*) *is equal to the logarithm of the topological tau-function of the integrable hierarchy of the topological type associated with* $M^n_{\mathbf{P}^N}$.

Recall (see above) that for $N = 0$ the hierarchy in question coincides with KdV, for $N = 1$ this is the extended Toda hierarchy; starting from $N = 2$ the integrable hierarchy is a new gadget of the theory of integrable systems.

Remark 28. The action of the Givental operator $\hat{G}_\infty(w)$ on the product of *topological* tau-functions

$$\hat{G}_\infty(w)\tau^{\mathrm{top}}_{\mathrm{KdV}}(\mathbf{t}^1;\epsilon)\dots\tau^{\mathrm{top}}_{\mathrm{KdV}}(\mathbf{t}^n;\epsilon)$$

is also well defined. Moreover, the result is a power series with respect to the new time variables. The coefficients of these power series depend on the point $w \in M$ of the Frobenius manifold. These series play an important role in the classification of semisimple cohomological field theories obtained by C. Teleman [64].

The above considerations suggest that the intrinsic structure of integrable hierarchies of the topological type is closely related to the topology of the Deligne–Mumford spaces. Let us formulate a more precise conjecture about such a relation. Among all differential equations for the total Gromov–Witten potential

$$\begin{aligned}
\mathcal{F}^X(\mathbf{t};\epsilon^2) &= \sum_{g\geq 0}\epsilon^{2g-2}\mathcal{F}^X_g(\mathbf{t}) \qquad (105)\\
\mathcal{F}^X_g(\mathbf{t}) &= \sum_m \sum_{\beta\in H_2(X;\mathbf{Z})} \frac{1}{m!}t^{\alpha_1,p_1}\dots t^{\alpha_m,p_m}\langle\tau_{p_1}(\phi_{\alpha_1})\dots\tau_{p_m}(\phi_{\alpha_m})\rangle_{g,\beta}\\
&\quad\times\langle\tau_{p_1}(\phi_{\alpha_1})\cdots\tau_{p_m}(\phi_{\alpha_m})\rangle_{g,\beta}\\
&:= \int_{[X_{g,m,\beta}]^{\mathrm{virt}}} ev_1^*(\phi_{\alpha_1})\wedge c_1^{p_1}(\mathcal{L}_1)\wedge\cdots\wedge ev_m^*(\phi_{\alpha_m})\wedge c_1^{p_m}(\mathcal{L}_m)\\
X_{g,m,\beta} &:= \left\{f:\left(C_g,x_1,\dots,x_m\right)\to X,\quad f_*[C_g]=\beta\in H_2(X;\mathbb{Z})\right\}
\end{aligned}$$

of a smooth projective variety X the *universal* identities are of particular interest. By definition they are those relations between Gromov–Witten invariants and their descendents

$$\langle\tau_{p_1}(\phi_{\alpha_1})\dots\tau_{p_m}(\phi_{\alpha_m})\rangle_{g,\beta}$$

that do not depend on X (cf. [49, 50]). Besides the already familiar WDVV (in genus 0) there are topological recursion relations for the descendents, and also the Getzler's universal identities [37] for genus 1 GW invariants etc. An example of non-universal differential equations for $\mathcal{F}^X$ is given by the Virasoro constraints. The coefficients of the Virasoro operators depend on the classical cohomology ring of X together with the first Chern class $c_1(X)$.

Let us proceed to formulation of our main conjecture that relates the theory of integrable PDEs with the theory of Gromov–Witten invariants and their descendents. For a smooth projective X denote $H^{\mathrm{alg}}(X)\subset H^*(X)$ the subspace generated by (k,k) forms (we do not impose the restriction $H^{\mathrm{odd}}(X)=0$). Introduce the differential ideal $I^{\mathrm{alg}}_{GW}(n)$ generated by polynomial identities for the derivatives of the form

$$\langle\!\langle\tau_{p_1}(\phi_{\alpha_1})\dots\tau_{p_m}(\phi_{\alpha_m})\rangle\!\rangle_g = \frac{\partial^m}{\partial t^{\alpha_1,p_1}\dots\partial t^{\alpha_m,p_m}}\mathcal{F}^X$$

with

$$\phi_{\alpha_i} \in H^{\mathrm{alg}}(X), \quad i = 1, \dots, m$$

for all $m \geq 0$ valid for *all* X with $\dim H^{\mathrm{alg}}(X) = n$.

Another differential ideal $I_{\mathrm{KdV}}(n)$ is generated by polynomial differential equations for the logarithmic derivatives of the tau-function τ_{top} valid for *an arbitrary* n-dimensional semisimple Frobenius manifold M^n.

Conjecture 29. For any $n \geq 0$

$$I_{\mathrm{KdV}}(n) = I^{\mathrm{alg}}_{GW}(n).$$

5 Critical Behaviour in Hamiltonian PDEs, the Dispersionless Case

The new integrable hierarchies described in the previous section are written as infinite formal expansions in ϵ. For practical applications of these PDEs one has to truncate them at some order in ϵ. The natural question arises: how do the properties of solutions depend on the truncation order? What part of these properties is *universal*, i.e., independent of the choice of a generic solution and possibly, on the choice of a Hamiltonian PDE?

The idea suggested by the author in [19] is to classify the types of *critical behavior* of solutions to Hamiltonian PDEs. By definition this is the behavior of a solution to the Hamiltonian PDE near the points of weak singularities (also called gradient catastrophes) of the dispersionless limit of the PDE. The idea of universality suggests that, up to simple transformations there exists only finite number of types of critical behavior.

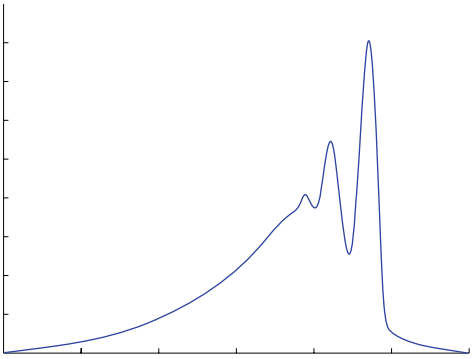

Fig. 2 Critical behavior in the KdV equation, cf. [71]

In the present section we will briefly describe the local structure of gradient catastrophes for the systems of first order Hamiltonian PDEs. In the next section

we will formulate and discuss the universality conjectured for Hamiltonian perturbations of these PDEs.

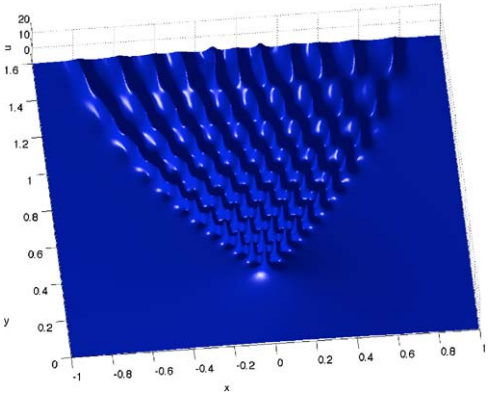

Fig. 3 Critical behavior in the focusing NLS equation; the graph of $u = |\psi|^2$ is shown

Solutions to hyperbolic systems typically have a finite life time. Let us begin with considering the simplest situation of the scalar nonlinear transport equation

$$v_t + a(v)v_x = 0. \tag{106}$$

As in Example 3 (106) can be considered as an integrable Hamiltonian system with the Hamiltonian and Poisson bracket of the form

$$H_f^0 = \int f(v)\,dx, \quad f''(v) = a(v), \quad \{v(x), v(y)\} = \delta'(x-y). \tag{107}$$

The solution $v = v(x,t)$ to the Cauchy problem $v(x,0) = v_0(x)$ for (106) exists till the time $t = t_0$ of *gradient catastrophe*. At this point $x = x_0$, $t = t_0$, $v = v_0$,

$$v(x,t) \to v_0, \qquad v_x(x,t) \to \infty \quad \text{for } (x,t) \to (x_0,t_0), \quad t < t_0.$$

The following statement is well known.

Theorem 30. *Up to shifts, Galilean transformations and rescalings near the point of gradient catastrophe the generic solution approximately behaves as the root* $v = v(x,t)$ *of cubic equation*

$$x = vt - \frac{v^3}{6}$$

(*bifurcation diagram of* A_3 *singularity*).

Proof The solution can be found by the *method of characteristics*:

$$x = a(v)t + b(v) \tag{108}$$

for an arbitrary smooth function $b(v)$. At the point of gradient catastrophe one has

$$\begin{aligned} x_0 &= a(v_0)t_0 + b(v_0) \\ 0 &= a'(v_0)t_0 + b'(v_0) \\ 0 &= a''(v_0)t_0 + b''(v_0) \end{aligned} \tag{109}$$

(an inflection point). We impose the *genericity assumption*

$$\kappa := -\left(a'''(v_0)t_0 + b'''(v_0)\right) \neq 0. \tag{110}$$

Introduce the new variables

$$\begin{aligned} \bar{x} &= x - a_0(t - t_0) - x_0 \\ \bar{t} &= t - t_0 \\ \bar{v} &= v - v_0. \end{aligned}$$

Here $a_0 = a(v_0)$, $a_0' := a'(v_0)$ etc. Rescaling

$$\bar{x} \mapsto \lambda \bar{x}, \qquad \bar{t} \mapsto \lambda^{\frac{2}{3}} \bar{t}, \qquad \bar{v} \mapsto \lambda^{\frac{1}{3}} \bar{v}, \tag{111}$$

substituting in $x = a(v)t + b(v)$ and expanding at $\lambda \to 0$ one obtains, after division by λ

$$\bar{x} = a_0' \bar{t} \bar{v} - \frac{1}{6}\kappa \bar{v}^3 + O\left(\lambda^{\frac{1}{3}}\right).$$

Similar arguments can be applied to the two component systems. We will consider here only the case of the nonlinear wave equation [20]

$$u_{tt} - \partial_x^2 P'(u) = 0 \tag{112}$$

for a given smooth function $P(u)$. Equation (112) is linear for a quadratic function $P(u)$; we assume therefore that

$$P'''(u) \neq 0.$$

The system (50) can be written in the Hamiltonian form

$$\begin{aligned} u_t &= \partial_x \frac{\delta H}{\delta v(x)} \\ v_t &= \partial_x \frac{\delta H}{\delta u(x)} \end{aligned} \tag{113}$$

with the Hamiltonian

$$H = \int \left[\frac{1}{2}v^2 + P(u)\right] dx. \tag{114}$$

The associated Poisson bracket is standard (see (14))

$$\{u(x), v(y)\} = \delta'(x - y). \tag{115}$$

The system is hyperbolic on the domain of convexity of $P(u)$,

$$(u, v) \in \mathbb{R}^2 \quad \text{such that} \quad P''(u) > 0 \tag{116}$$

and elliptic when $P(u)$ becomes concave. Denote $r_\pm$ the Riemann invariants of the system,

$$r_\pm = v \pm Q(u), \quad \text{where } Q'(u) = \sqrt{P''(u)}. \tag{117}$$

The equations (28) for the conserved quantities for (113) reduce to

$$f_{uu} = P''(u) f_{vv}. \tag{118}$$

The generic solution $(u(x, t), v(x, t))$ can be locally determined from the implicit function equations

$$\begin{aligned} x &= f_u(u, v) \\ t &= f_v(u, v) \end{aligned} \tag{119}$$

The points (x_0, t_0, u_0, v_0) of catastrophe are determined from the system

$$\left.\begin{aligned} x_0 &= f_u(u_0, v_0) \\ t_0 &= f_v(u_0, v_0) \\ 0 &= f_{uv}^2(u_0, v_0) - P''(u_0) f_{vv}^2(u_0, v_0) \end{aligned}\right\}. \tag{120}$$

Let us first consider the hyperbolic catastrophe, $P''(u_0) > 0$. Let (x_0, t_0, u_0, v_0) be the first catastrophe, i.e., the solution is smooth for $t < t_0$ for sufficiently small $|x - x_0|$. At a generic critical point only one of the Riemann invariants blows up. Let it be r_-. Introduce the shifted characteristic variables

$$\bar{x}_\pm = (x - x_0) \pm \sqrt{P''(u_0)}(t - t_0) \tag{121}$$

and shifted Riemann invariants

$$\bar{r}_\pm = r_\pm - r_\pm(u_0, v_0).$$

Theorem 31. *Up to rescalings near the first point of hyperbolic gradient catastrophe the generic solution to the nonlinear wave equation approximately behaves as the solution to the system*

$$\begin{aligned} \bar{x}_+ &= \bar{r}_+ \\ \bar{x}_- &= \bar{r}_+ \bar{r}_- - \frac{1}{6}\bar{r}_-^3. \end{aligned} \tag{122}$$

Observe that (122) is one of the normal forms of singularities of smooth maps $\mathbb{R}^2 \to \mathbb{R}^2$ classified by H. Whitney in [67].

Let us now consider elliptic critical points (120), $P''(u_0) < 0$. In this case the Riemann invariants (117) are complex conjugate. So they have a simultaneous blow up. Therefore the critical points are located at isolated points (x_0, t_0) of the (x, t) plane. In order to describe the local structure of the generic solution near the critical point let us introduce complex variables

$$z = (x - x_0) + ic_0(t - t_0), \qquad w = (v - v_0) + ic_0(u - u_0) \tag{123}$$

where

$$c_0 = \sqrt{-P''(u_0)}.$$

Theorem 32. *Near the point of elliptic gradient catastrophe the generic solution to the nonlinear wave equation approximately behaves as the solution to the complex quadratic equation*

$$z = \frac{1}{2}a_0 w^2, \quad a_0 = f_{uvv}(u_0, v_0) + ic_0 f_{vvv}(u_0, v_0) \neq 0. \tag{124}$$

Separating the real and imaginary parts of (124) one obtains a description of the critical behavior (124) in terms of the so-called elliptic umbilic catastrophe [65].

Similar description can be obtained for the critical behavior of solutions to any of the commuting flows

$$\begin{aligned} u_s &= \partial_x f_v(u, v) \\ v_s &= \partial_x f_u(u, v) \end{aligned} \tag{125}$$

where $f = f(u, v)$ is an arbitrary solution to (118). The details can be found in [20].

Example 33. Consider the (focusing) nonlinear Schrödinger equation

$$i\psi_t + \frac{1}{2}\psi_{xx} + |\psi|^2\psi = 0 \tag{126}$$

written in the coordinates

$$u = |\psi|^2, \qquad v = \frac{1}{2i}\left(\frac{\psi_x}{\psi} - \frac{\bar{\psi}_x}{\bar{\psi}}\right),$$

i.e.,

$$\begin{aligned} &u_t + (uv)_x = 0 \\ &v_t + vv_x - u_x = \frac{1}{4}\left(\frac{u_{xx}}{u} - \frac{1}{2}\frac{u_x^2}{u^2}\right)_x. \end{aligned}$$

The dispersionless limit

$$\begin{aligned} u_t + (uv)_x &= 0 \\ v_t + vv_x - u_x &= 0 \end{aligned} \tag{127}$$

is an infinitesimal symmetry of the nonlinear wave equation with

$$P(u) = -u(\log u - 1).$$

The system (127) is of elliptic type due to obvious inequality $u > 0$. So its generic critical points have the form (124).

For $n \geq 3$ it is not difficult to see that critical points of a generic solution to any *integrable* first order quasilinear system can be essentially described by the same singularities of the types (122) or (124). At the moment we do not have a classification of the singularity types for solutions to non integrable quasilinear systems.

6 Universality in Hamiltonian PDEs

In the previous section we classified the types of generic critical behavior of solutions to dispersionless Hamiltonian PDEs of low order. In the present section we will study the effects of higher order Hamiltonian perturbations. It turns out that, the above list of types of critical behavior given in terms of algebraic functions has to be replaced by another list given in terms of particular Painlevé transcendents and their higher order generalizations.

Let us begin with describing one of these special functions.

Consider the following fourth order ODE for the function $U = U(X)$ depending on T as on the parameter

$$X = TU - \left[\frac{1}{6}U^3 + \frac{1}{24}\left(U'^2 + 2UU''\right) + \frac{1}{240}U^{IV}\right]. \tag{128}$$

Equation (128) is usually considered as the fourth order analogue of the classical Painlevé-I equation P_I (see below); it is denoted P_I^2. The following result was proved by T. Claeys and M. Vanlessen [10].

Theorem 34. *For any $T \in \mathbb{R}$ there exists a solution to* (128) *real and smooth for all real X. For large $|X|$ the solution has the asymptotic behaviour*

$$U \sim -(6X)^{1/3}, \quad |X| \to \infty. \tag{129}$$

Actually, the solution of interest has been constructed for all real X and T by solving certain Riemann–Hilbert problem depending on X and T as on the parameters. The main difficulty was to prove existence of a solution to the Riemann–Hilbert problem for all $(X, T) \in \mathbb{R}^2$. This solution will be denoted $U(X, T)$.

The conjectural existence of the smooth solution to the ODE4 has been first discussed (for the particular value $T = 0$) by É. Brézin, G. Marinari, A. Parisi [6] and by G. Moore [57] in the setting of the theory of random matrices. Within the class (129) the uniqueness can be established using results of G. Moore [57] and A. Menikoff [54].

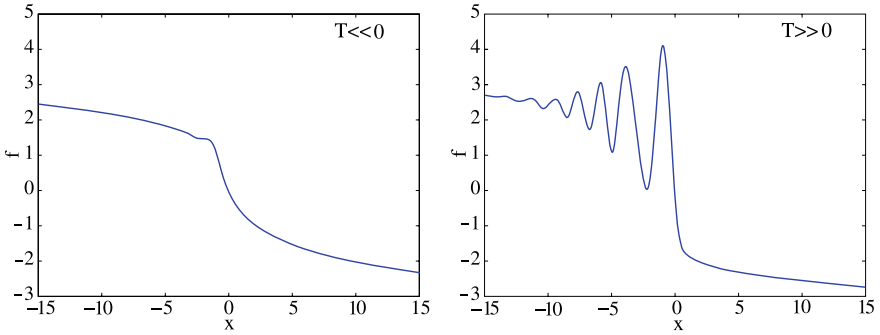

Fig. 4 The solution $U(X, T)$ to the ODE (128) for two instants of time T

Importance of the smooth solution to the ODE4 for the so-called *Gurevich–Pitaevsky* solution to KdV was discussed by B. Suleimanov [62] and V. Kudashev and B. Suleimanov [48].

Remark 35. A somewhat stronger conjecture was formulated by the author in [19]. It says that for any real T there exists a *unique* real solution to (128) smooth for all real X. No assumptions about the asymptotic behavior are needed. This conjecture remains open.

We are now ready to formulate, following [19], the Universality Conjecture about critical behavior of solutions to a generic Hamiltonian perturbations

$$u_t + \partial_x \frac{\delta H_f^\epsilon}{\delta u(x)} \equiv u_t + a(u)u_x + O(\epsilon^2) = 0, \quad H_f^\epsilon = H_f^0 + O(\epsilon^2) \tag{130}$$

of the scalar hyperbolic equation (106). Recall that all these perturbations have been classified in (24). Consider the solution $u(x, t; \epsilon)$ to (130) that tends to a solution $v(x, t)$ as $\epsilon \to 0$ to the unperturbed equation (106) for sufficiently small $t < t_0$. Assume that $v(x, t)$ is smooth for $t < t_0$ for all x with sufficiently small $x - x_0$ having a point of gradient catastrophe at $(x = x_0, t = t_0, v = v_0)$.

Conjecture 36. (1) For sufficiently small $\epsilon > 0$ and $|x - x_0|$ there exists a positive δ such that the solution $u(x, t; \epsilon)$ can be locally smoothly extended for $t < t_0 + \delta$.

(2) Near the point (x_0, t_0) it behaves in the following way

$$u \simeq v_0 + \left(\frac{\epsilon^2 c_0}{\kappa^2}\right)^{1/7} U\left(\frac{x - a_0(t - t_0) - x_0}{(\kappa c_0^3 \epsilon^6)^{1/7}}; \frac{a_0'(t - t_0)}{(\kappa^3 c_0^2 \epsilon^4)^{1/7}}\right) + O\left(\epsilon^{4/7}\right) \tag{131}$$

where

$$a_0 = a(v_0), \qquad a_0' = a'(v_0),$$

c_0 and κ are some nonzero constants, $U(X, T)$ the solution to (128) described in Theorem 34.

We will not reproduce here the arguments of [19] supporting this conjecture. It was analyzed numerically by T. Grava and C. Klein [42]. A rigorous proof of the conjecture for solutions to the KdV equation with analytic rapidly decreasing initial data was recently obtained by T. Claeys and T. Grava [9] by using the so-called steepest descent method, due to P. Deift and X. Zhou (see in [13]).

Remarkably, the same special function $U(X, T)$ appears in the description of the critical behavior of solutions to second order Hamiltonian systems near a hyperbolic critical point. We will give a sketch of the following Universality Conjecture for Hamiltonian perturbations of the nonlinear wave equation (112) inspired by results of [20].

Conjecture 37. Let $r_\pm$ and $x_\pm$ be as in (117), (121). Then for a solution to a generic Hamiltonian perturbation of (112) near the generic critical point of the form (122) one has

$$\begin{aligned} r_+ &\simeq r_+^0 + cx_+ + \alpha_+ \epsilon^{4/7} U'' \left(a\epsilon^{-6/7} x_-; b\epsilon^{-4/7} x_+ \right) + \mathcal{O}\left(\epsilon^{6/7}\right) \\ r_- &\simeq r_-^0 + \alpha_- \epsilon^{2/7} U \left(a\epsilon^{-6/7} x_-; b\epsilon^{-4/7} x_+ \right) + \mathcal{O}\left(\epsilon^{4/7}\right) \end{aligned} \tag{132}$$

where $U = U(X; T)$ is the same solution described in Theorem 34.

Proof of this conjecture remains an open problem. Observe recent result of [11] about asymptotics in Hermitean random matrices near singular edge points: for the recurrence coefficients

$$\begin{aligned} a_n(s,t) &= a_n^0 + \frac{1}{2} c n^{-2/7} U(c_1 n^{6/7} s, c_2 n^{4/7} t) + O\left(n^{-3/7}\right) \\ b_n(s,t) &= b_n^0 + c n^{-2/7} U(c_1 n^{6/7} s, c_2 n^{4/7} t) + O\left(n^{-3/7}\right). \end{aligned}$$

This result support Conjecture 37 for the case of solutions to equations of Toda hierarchy with some particular initial data. Also numerical results obtained in the beginning of '90s in the theory of random matrices (see Fig. 5) qualitatively support Conjecture 37.

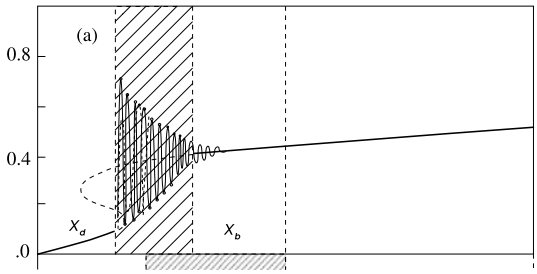

Fig. 5 Oscillatory behavior of correlation functions in the random matrix models, after [46]. The oscillatory zone corresponds to the two-cut region

We will now introduce another special function needed for the description of the critical behavior near *elliptic* critical points. The special function in question is defined as a particular solution to the classical Painlevé-I (P_I) equation for the function $W = W(Z)$, $Z \in \mathbb{C}$

$$W'' = 6W^2 - Z. \tag{133}$$

It is known that any solution to P_I is a meromorphic function on the complex plane. The following result was proved in 1913 by P. Boutroux [5].

Theorem 38. (1) *Poles of a generic solution to P_I accumulate along five rays*

$$\arg Z = \frac{2\pi n}{5}, \quad n = 0, \pm 1, \pm 2. \tag{134}$$

(2) *For any three consecutive rays there exists a* unique *so-called* tritronquée *solution such that the lines of poles truncate along these three rays for large $|Z|$.*

Let us consider the *tritronquée* solution $W_0(Z)$ associated with the triple of rays (134) with $n = 0$ and $n = \pm 1$. Due to Boutroux theorem this solution has at most finite number of poles in the sector

$$|\arg Z| < \frac{4\pi}{5} - \delta$$

for any positive δ. In [28] arguments were found suggesting the following

Conjecture 39. The tritronquée solution $W_0(Z)$ is holomorphic in the sector

$$|\arg Z| < \frac{4\pi}{5}. \tag{135}$$

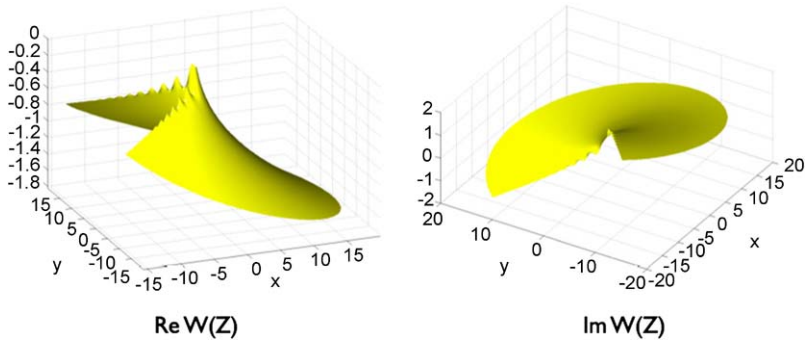

Fig. 6 The *tritronquée* solution $W(Z)$ to the P_I equation in the sector $|\arg Z| < \frac{4\pi}{5}$

We are now ready to formulate the Universality Conjecture for the critical behavior of solutions to Hamiltonian perturbations to the nonlinear wave equation (112) near a generic elliptic gradient catastrophe point.

Conjecture 40. Let w and z be as in (123). Then for a solution to a generic Hamiltonian perturbation of (112) near the generic critical point of the form (124) one has

$$w \simeq w^0 + \alpha\epsilon^{2/5} W_0\left(\epsilon^{-4/5} z\right) + \mathcal{O}\left(\epsilon^{4/5}\right) \tag{136}$$

for some nonzero complex constants α, β depending on the choice of the solution.

The complex constant β is such that the argument of the *tritronquée* solution $W_0(Z)$ belongs to the sector $|\arg Z| < \frac{4\pi}{5}$ for any $x \in \mathbb{R}$ for sufficiently small $|t - t_0|$. The conjecture first appeared in [28] in the description of the critical behaviour in the focusing NLS equation (127). It remains completely open, as well as the previous conjecture about the *tritronquée* solution to P_I.

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Lattice Supersymmetry from the Ground Up

Paul Fendley and Kareljan Schoutens

Abstract This talk summarizes a series of papers defining and analyzing lattice models with supersymmetry. These models describe strongly-interacting spinless fermions hopping on any lattice or graph. Computing the Witten index and the cohomology of the supersymmetry generator Q allows us to understand a great deal about the ground state. In all one-dimensional and some two-dimensional cases this allows the number and density of the ground states to be found exactly. In two dimensions and up, the ground-state entropy is extensive for generic lattices.

Supersymmetry is an exceptionally powerful theoretical tool. As thousands of papers have demonstrated, exact computations can often be done in supersymmetric field theory and string theory, even when the theories are strongly interacting. In a series of papers [5, 4, 6, 3], we develop a new tool: a lattice model with sypersymmetry. This model can be defined on any lattice in any dimension.

In our models the supersymmetry is akin to the "spacetime" supersymmetry arising in particle physics: the algebra of the supersymmetry generators also involves the Hamiltonian as well. Since these models are defined on the lattice, the supersymmetry is not that of a full Lorentz-invariant supersymmetric field theory, since that supersymmetry algebra involves translations as well.

Our strategy is thus much more analogous to that used in condensed matter physics than that of particle physics. Instead of picking some Lorentz-invariant spacetime supersymmetric field theory and discretizing it, we introduce simple lattice models whose superalgebra defines the Hamiltonian. By construction, these models are strongly interacting, but because of the supersymmetries, we can then

Paul Fendley
Department of Physics, University of Virginia, Charlottesville, VA 22904-4714, USA, e-mail: fendley@rockpile.phys.virginia.edu

Kareljan Schoutens
Institute for Theoretical Physics, University of Amsterdam, Valckenierstraat 65, 1018 XE Amsterdam, The Netherlands, e-mail: kjs@science.uva.nl

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derive exact and rigorous results for the ground state. We find a wide variety of interesting behavior, some of which I will outline here.

The Hamiltonian we construct has $\mathcal{N} = 2$ supersymmetry, meaning that it commutes with two nilpotent fermionic generators denoted Q and $Q^\dagger$. We require that Q is nilpotent: $Q^2 = (Q^\dagger)^2 = 0$. This means that both Q and $Q^\dagger$ commute with the Hamiltonian H defined by

$$H = \{Q, Q^\dagger\}. \tag{1}$$

Such a Hamiltonian has eigenvalues $E \geq 0$. All states $|g\rangle$ with $E = 0$ must be singlets: $Q|g\rangle = Q^\dagger|g\rangle = 0$. Conversely, all singlets must have $E = 0$. All the other eigenstates of H can be decomposed into doublets under the supersymmetry, and conversely any doublet representation is an eigenstate. This is simple to prove: a doublet consists of two states $|s\rangle$, $Q|s\rangle$, where $Q^\dagger|s\rangle = 0$. It follows from the definition of H and the nilpotency of Q that both of these states are eigenstates of H with the same eigenvalue.

To define a supersymmetric lattice model therefore requires only finding an fermionic operator Q which squares to zero. However, most such models will be trivial, too complicated, or have non-local interactions. An example of the first comes from considering degrees of freedom defined by allowing a spinless fermion on the sites i of any lattice or graph. The fermion is created by the operator $c_i^\dagger$ obeying the usual anticommutator $\{c_i, c_j^\dagger\} = \delta_{ij}$. The space of states of the theory is given by operating with the $c_i^\dagger$ on the vacuum. Then it is easy to check that the operator $\sum_i c_i^\dagger$ indeed squares to zero. However, the resulting Hamiltonian is trivial: H is simply the number of sites.

Thus we must make the model a little more complicated to get something nontrivial. Our papers mainly deal with the case where the Hilbert space remains that of a single species of spinless fermion, but with the additional restriction that the fermions have hard cores. This means that fermions are not allowed on neighboring sites. We define the projection operator $\mathscr{P}_{\langle i\rangle}$ to be the operator which requires all sites neighboring i to be empty:

$$\mathscr{P}_{\langle i\rangle} = \prod_{j \text{ next to } i} (1 - c_j^\dagger c_j) \tag{2}$$

Thus entire space of states is built up by acting with all the $c_i^\dagger \mathscr{P}_{\langle i\rangle}$. The supersymmetry operators are then defined by

$$Q = \sum_i c_i^\dagger \mathscr{P}_{\langle i\rangle}, \qquad Q^\dagger = \sum_i c_i \mathscr{P}_{\langle i\rangle}. \tag{3}$$

It is easy to verify that $Q^2 = 0$: the only potentially non-zero terms are of the form $c_i^\dagger \mathscr{P}_{\langle i\rangle} c_j^\dagger \mathscr{P}_{\langle j\rangle}$ for i and j nearest neighbors, but in this case $\mathscr{P}_{\langle i\rangle} c_j^\dagger = 0$.

With these supercharges, the Hamiltonian is

$$H = \sum_i \sum_{j \text{ next to } i} \mathscr{P}_{\langle i \rangle} c_i^\dagger c_j \mathscr{P}_{\langle j \rangle} + \sum_i \mathscr{P}_{\langle i \rangle} \tag{4}$$

where we used the fact that $(\mathscr{P}_{\langle i \rangle})^2 = (\mathscr{P}_{\langle i \rangle})$. The first term in the Hamiltonian allows fermions to hop to neighboring sites on the lattice, with the projectors ensuring the hard-core repulsion. The second term includes a chemical potential and a repulsive potential for fermions two sites from each other. The latter term has a more conventional form on a lattice where every site has z nearest neighbors:

$$\sum_i \mathscr{P}_{\langle i \rangle} = N - zF + \sum_i V_{\langle i \rangle} \tag{5}$$

where $V_{\langle i \rangle} + 1$ is the number of particles adjacent to i, unless there are none, in which case $V_{\langle i \rangle} = 0$. The operator $F = \sum_i d_i^\dagger d_i$ counts the number of fermions. So in addition to the hard core, the Hamiltonian includes a hopping term, a constant (which we keep to ensure ground states have $E = 0$), a chemical potential z, and repulsive interactions between fermions two sites apart. Note that this model has have a fermion-number symmetry generated by

$$F = \sum_i c_i^\dagger c_i,$$

so that $[F, Q] = Q$. Thus the fermion-number generator F indeed counts the number of fermions.

We have analyzed this model on a one-dimensional chain in depth. It has the additional nice feature of being integrable [4], and the supersymmetry turns out to complement the integrability nicely. The model turns out to be closely related to the XXZ spin chain at anisotropy $\Delta = -1/2$. In fact, the ground state of our model in one dimension has a number of striking properties, closely related to those arising in studies of the Razumov-Stroganov conjecture; see [1] and references therein. Even though Lorentz invariance was not required initially, it turns out to be a consequence: the field theory describing the continuum limit is the first $N = (2, 2)$ superconformal minimal model [5]. However, other one-dimensional models with supersymmetry discussed in [4] do not always yield Lorentz-invariant field theories.

We have already noted several of the consequences of supersymmetry: positive energy and excited-state pairing. To go further, we use two mathematical tools to study the $E = 0$ ground states of (4). The first is the *Witten index* W [10]. It is similar to the partition function, but includes a minus sign for each fermion:

$$W = \mathrm{tr}\big[(-1)^F e^{-\beta H}\big]. \tag{6}$$

W is a lower bound on the number of ground states: it is the difference of the number of bosonic ground states and the number of fermionic ground states. This is because all energy eigenstates with $E > 0$ form boson/fermion doublets of the same energy E but opposite $(-1)^F$. The states in a doublet contribute to W with opposite signs and cancel, leaving only the sum of $(-1)^F$ over the ground states.

This argument shows that W is independent of β, so we can evaluate it in the $\beta \to 0$ limit, where every state contributes with weight $(-1)^F$. We compute this by dividing the lattice into two sublattices S_1 and S_2; we fix a configuration on S_1, and sum $(-1)^F$ for the configurations on S_2. Then we sum the results over the configurations on S_1. For a periodic chain with $N = 3j$ sites, we take S_2 to be every third site, and the remaining sites S_1. Then the sum over configurations on any site on S_2 vanishes unless at least one of the adjacent sites on S_1 is occupied.

$$\sum_{\square=\circ,\bullet} (\circ\square\circ) = \circ\bullet\circ + \circ\circ\circ = (-1) + 1 = 0.$$

Because of the hard-core restriction on the fermions and the periodic boundary conditions, there are only two such configurations:

$$\begin{aligned} |\alpha\rangle &\equiv \cdots \bullet \square \circ \bullet\square \circ \bullet\square \circ \bullet\square \circ \bullet\square \circ \bullet\square \circ \bullet\square \circ \cdots \\ |\gamma\rangle &\equiv \cdots \circ \square \bullet \circ\square \bullet \circ\square \bullet \circ\square \bullet \circ\square \bullet \circ\square \bullet \circ\square \bullet \cdots \end{aligned} \tag{7}$$

where the square represents an empty site on S_2. Both $|\alpha\rangle$ and $|\gamma\rangle$ have $f = N/3$, so $W = 2(-1)^f$, requiring that are at least two ground states.

The second tool we use is the computation of the *cohomology* H_Q of the operator Q. This tool is even more powerful, allowing us to obtain not just a lower bound, but rather the precise number of ground states, and the fermion number of each. The cohomology is the vector space of states which are annihilated by Q but which are not Q of something else (in mathematical parlance, these states are closed but not exact) [2]. Since $Q^2 = 0$, any state which is Q of something is annihilated by Q. Two states $|s_1\rangle$ and $|s_2\rangle$ are said to be in the same cohomology class if $|s_1\rangle = |s_2\rangle + Q|s_3\rangle$ for some state $|s_3\rangle$.

The non-trivial cohomology classes are in one-to-one correspondence with the $E = 0$ ground states [5]. To see this, consider an energy eigenstate $|E\rangle$ with eigenvalue $E > 0$. If $Q|E\rangle \neq 0$, then it is not in any cohomology class. If $Q|E\rangle = 0$ but $H|E\rangle \neq 0$, then $|E\rangle = Q(Q^\dagger|E\rangle/E)$. This is in the trivial cohomology class, so only the $E = 0$ ground states have non-trivial cohomology. Because they are annihilated by both Q and $Q^\dagger$, linearly independent $E = 0$ ground states must be in different cohomology classes. Precisely, the dimension of the vector space of ground states (the "number" of ground states) is the same as that of the cohomology. Since F commutes with the Hamiltonian, the cohomology class and the corresponding ground state have the same fermion number.

We find the exact number of ground states by computing the cohomology H_Q by using a *spectral sequence*. A useful theorem is the "tic-tac-toe" lemma of Ref. [2]. This says that under certain conditions, the cohomology H_Q for $Q = Q_1 + Q_2$ is the same as the cohomology of Q_1 acting on the cohomology of Q_2. In an equation, $H_Q = H_{Q_1}(H_{Q_2}) \equiv H_{12}$. As with our computation of W, H_{12} is found by first fixing the configuration on all sites on the sublattice S_1, and computing the cohomology H_{Q_2}. Then one computes the cohomology of Q_1, acting not on the full space of states, but only on the classes in H_{Q_2}. A sufficient condition for the lemma

to hold is that all non-trivial elements of H_{12} have the same f_2 (the fermion number on S_2).

Having introduced the mathematical tools necessary, we now turn to the study of our spinless-fermion model on two-dimensional lattices. We find that generically, there is an *extensive ground state entropy*: the number of ground states increases exponentially with the size of the system. This indicates that the system is frustrated; we will explain how in the following.

The systematics of the one-dimensional case quickly extend to lattices of type Λ_3, which are obtained from any lattice (or even graph) Λ by putting two additional sites on every link. Letting S_1 be the original sites of Λ and S_2 the added sites, the only states in H_{Q_2} and H_{12} are the two where S_1 is completely full, and completely empty. The first gives an $E = 0$ ground state with $f = N_\Lambda$ (the number of sites of Λ), while the latter gives an $E = 0$ state with $f = L_\Lambda$ (the number of links in Λ), with a possible exception when $L_\Lambda = N_\Lambda - 1$. When Λ is the square lattice, the two ground states on Λ_3 have filling $f = N/5$ and $f = 2N/5$. Lattices of type Λ_3 are the only two-dimensional ones we know of where the number of ground states does not grow with the size of the lattice.

Another exceptional case is the octagon-square lattice on the right of Fig. 1. We take L rows and M columns of squares (hence $N = 4LM$ sites). Let S_1 consist of the leftmost site on every square. Then H_{Q_2} is trivial unless all the M sites on S_1 in a given row either all are occupied, or all are empty. There are $2^L - 1$ such configurations which have at least one row in S_1 occupied. Because of the hard core, all the sites of S_2 adjacent to an occupied site on S_1 cannot be filled, and the remaining sites form independent open chains of length a multiple of 3. Such an open chain has just one element of H_{Q_2}, so each of these $2^L - 1$ configurations correspond to one element of H_{Q_2} and H_{12}. Now consider the configuration where all sites on S_1 are empty, so that the sites on S_2 form M periodic chains, each of length $3L$. We showed above that H_{Q_2} for *each* of these chains has *two* independent elements. Thus H_{Q_2} and H_{12} are of dimension $2^L + 2^M - 1$. Applying the tic-tac-toe lemma to this case is more involved, but the conclusion is that there are $2^L + 2^M - 1$ ground states, each with $N/4$ fermions.

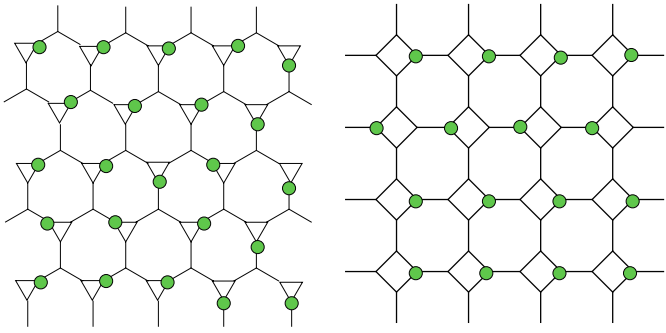

Fig. 1 Configurations obeying the 3-rule on the martini and the octagon-square lattices

We believe that on the octagon-square lattice, the model exhibits a combination of Wigner-crystal order with frustration. There are $2^L + 2^M$ configurations of $N/4$ particles which satisfy our heuristic 3-rule. 2^L of them are of the form displayed in Fig. 1: one can shift all the particles in a given row without violating the rule. This illustrates how frustration arises: in each row one can shift all the particles without violating the 3-rule. Likewise, 2^M of them have particles on the top or bottom of each square. For mysterious reasons, the state with $(k_x, k_y) = 0$ is not a ground state, but we believe the remaining $2^L + 2^M - 1$ ordered states dominate the actual ground states. In further support of this claim, we analyze the discrete symmetries commuting with Q. If a given element of the cohomology spontaneously breaks such a symmetry, the corresponding ground state will break it too. The ground states have spontaneously-broken parity symmetries like the Wigner crystal states in Fig. 1. Again like the crystal, all but one of the $2^L - 1$ ground states first considered spontaneously break translation symmetry in the vertical direction but not the horizontal; $2^M - 2$ of the remaining ground states spontaneously break translation symmetry in the horizontal direction. Moreover, the number of ground states here can be changed by requiring that just one site anywhere on the lattice be occupied. Consider the octagon-square lattice with one site on S_1 and its three neighbors on S_2 removed; this is equivalent to demanding that there be a particle on this S_1 site. On this lattice there are just 2^{L-1} ground states. Only in an ordered system should this type of change occur.

These arguments give a hint that there are unusual fractionally-charged excitations in this two dimensional model. On the one-dimensional chain, excitations have fermion number $1/2$ [4]. These excitations can be understood heuristically as corresponding to kinks separating regions which locally look like the two possible ground states. For the octagon square lattice, a similar situation exists, which is illustrated in Fig. 2. There are two defects (i.e. two places particles are not three sites apart),

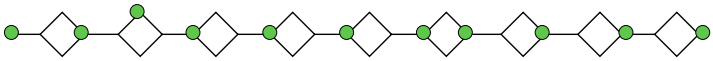

Fig. 2 Fractional charge?

but only one extra fermion relative to the ground state. Thus this is a strong hint that there are charge-$1/2$ excitations which are deconfined in one direction, confined in the other. Unfortunately, the two-dimensional model is not integrable like the chain is, so whether these excitations remain in the continuum limit (i.e. are deconfined) is still an open question.

The Λ_3 and octagon-square lattices are exceptional: on most other lattices we have studied the ground-state entropy is extensive. In many cases (including the triangular, hexagonal and Kagomé lattices), this can be seen by computing the Witten index W as a function of the size of the lattice. Employing a row-to-row transfer matrix T_M, the index for $M \times L$ unit cells is expressed as $W_{L,M} = \mathrm{tr}[(T_M)^L]$. We found by exact diagonalization that the largest eigenvalues $\lambda_M^{\max}$ of the T_M here behave as $\lambda_M^{\max} \propto \lambda^M$, with $|\lambda| > 1$. Clearly, the absolute value $|\lambda|$ sets a

lower bound on the ground-state entropy per lattice site. For n sites per unit cell, $S_{\rm GS}/N \geq \ln|W_{L,M}|/(nML) \sim \ln|\lambda|/n$. For the triangular lattice, $S_{\rm GS}/N \geq 0.13$ [9, 6].

For the nonagon-triangle "martini" lattice shown in the left half of Fig. 1, the extensive ground-state entropy can be exactly computed. The martini lattice is formed by replacing every other site on a hexagonal lattice with a triangle. To find the ground states, take S_1 to be the sites on the triangles, and S_2 to be the remaining sites. As with the chain, H_{Q_2} vanishes unless every site in S_2 is adjacent to an occupied site on some triangle. The non-trivial elements of H_{Q_2} therefore must have precisely one particle per triangle, each adjacent to a different site on S_2. This is because a triangle can have at most one particle on it, and (with appropriate boundary conditions) there are the same number of triangles as there are sites on S_2. A typical element of H_{Q_2} is shown in Fig. 1. One can think of these as "dimer" configurations on the original honeycomb lattice, where the dimer stretches from the site replaced by the triangle to the adjacent non-triangle site. Each close-packed hard-core dimer configuration is in H_{12}, and by the tic-tac-toe lemma, it corresponds to a ground state. The number of such ground states $e^{S_{\rm GS}}$ is therefore equal to the number of such dimer coverings of the honeycomb lattice, which for large N is [8, 11]

$$\frac{S_{\rm GS}}{N} = \frac{1}{\pi}\int_0^{\pi/3} d\theta \ln[2\cos(\theta)] = 0.16153\ldots \tag{8}$$

The frustration here clearly arises because there are many ways of satisfying the 3-rule.

This extensive ground-state entropy appears to be generic behavior. The Witten index provides a lower bound on the number of ground states, and it is easy to compute numerically by using a transfer matrix (it is a purely two-dimensional classical quantity). Numerics on the Witten index [9] clearly indicate extensive behavior for the triangular, honeycomb and other lattices Although the martini lattice does have generic behavior in its extensive ground-state entropy, it also is special in that all the ground state have the same number of fermions. This does not appear to be the case for generic two-dimensional lattices, as becomes apparent by studying the cohomology for small lattices in detail.

The square lattice turns out to be the most peculiar case. It is like the octagon-square case in that its ground-state entropy grows with the linear dimensions of the system, but like the generic case in that the filling fraction of the ground state varies over a continuous range, here between 1/5 and 1/4 filling. The Witten index itself has a number of striking properties [6], and after this talk was given, many new developments have occurred, summarized in [7].

Our exact results indicate that there is a new kind of exotic phase for itinerant fermions on a two-dimensional lattice with strong interactions. This "superfrustrated" state exhibits an extensive ground-state entropy, and occurs because supersymmetry ensures a perfect balance between competing terms in the Hamiltonian. Patterns with charge order can be distinguished in various limits and on spe-

cial lattices, but the effect of (approximate) supersymmetry in general is that defects between different domains come at zero (very low) energy cost.

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Convergence of Symmetric Trap Models in the Hypercube

L.R.G. Fontes* and P.H.S. Lima**

Abstract We consider symmetric trap models in the d-dimensional hypercube whose ordered mean waiting times, seen as weights of a measure in $\mathbb{N}^*$, converge to a finite measure as $d \to \infty$, and show that the models suitably represented converge to a K process as $d \to \infty$. We then apply this result to get K processes as the scaling limits of the REM-like trap model and the Random Hopping Times dynamics for the Random Energy Model in the hypercube in time scales corresponding to the *ergodic* regime for these dynamics.

1 Introduction

Trap models have been proposed as qualitative models exhibiting localization and aging (see [13, 7] for early references). In the mathematics literature there has recently been an interest in establishing such results for a varied class of such models (see [11, 4, 5] and references therein). In particular, it has been recognized that scaling limits play an important role in such derivations (see [11, 2, 10, 6] and references therein). It may be argued that such phenomena correspond to related phenomena exhibited by limiting models.

In this paper we consider symmetric trap models in the hypercube whose mean waiting times converge as a measure to a finite measure as the dimension diverges,

L.R.G. Fontes
Instituto de Matemática e Estatística, Universidade de São Paulo, Rua do Matão 1010, Cidade Universitária, 05508-090 São Paulo SP, Brasil, e-mail: lrenato@ime.usp.br

P.H.S. Lima
Instituto de Matemática e Estatística, Universidade de São Paulo, Rua do Matão 1010, Cidade Universitária, 05508-090 São Paulo SP, Brasil, e-mail: plima@ime.usp.br

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and show that these models converge weakly. We then apply this result to establish the scaling limits of two dynamics in the hypercube, namely the REM-like trap model and the Random Hopping Times dynamics for the Random Energy Model, in time scales corresponding to the ergodic regime for these dynamics.

1.1 The Model

Let $\mathscr{H}$ denote the d-dimensional hypercube, namely $\mathscr{H}$ is the graph $(\mathscr{V}, \mathscr{E})$ with

$$\mathscr{V} = \{0,1\}^d,$$
$$\mathscr{E} = \{(v, v') \in \mathscr{V} \times \mathscr{V} : |x - x'| = 1)\},$$

where $|v - v'| = \sum_{i=1}^{d} |v(i) - v'(i)|$ is the Hamming distance in $\mathscr{V}$.

We will consider symmetric trap models in $\mathscr{H}$, namely continuous time, space inhomogeneous, simple random walks in $\mathscr{H}$, whose transition probabilities (from each site of $\mathscr{H}$ to any of its d nearest neighbors) are uniform. Let $\gamma^d = \{\gamma_v^d,\ v \in \mathscr{V}\}$ denote the set of mean waiting times characterizing the model.

We will map $\mathscr{V}$ onto the set $\mathscr{D} := \{1, \ldots, 2^d\}$ by enumerating $\mathscr{V}$ in decreasing order of γ^d (with an arbitrary tie breaking rule), and then consider X^d, the mapped process. Let

$$\tilde{\gamma}^d = \{\tilde{\gamma}_x^d,\ x \in \mathscr{D}\} \tag{1}$$

denote the enumeration in decreasing order of γ^d, and view it as a finite measure in $\mathbb{N}^* = \{1, 2, \ldots\}$, the positive natural numbers.

We next consider a class of processes which turns out to contain limits of trap models in $\mathscr{H}$ as $d \to \infty$, as we will see below. Let $\mathscr{N} = \{(N_t^{(x)})_{t \geq 0},\ x \in \mathbb{N}^*\}$ be i.i.d. Poisson processes of rate 1, with $\sigma_j^{(x)}$ the j-th event time of $N^{(x)}$, $x \in \mathbb{N}^*$, $j \geq 1$, and let $\mathscr{T} = \{T_0;\ T_i^{(x)},\ i \geq 1, x \in \mathbb{N}^*\}$ be i.i.d. exponential random variables of rate 1. $\mathscr{N}$ and $\mathscr{T}$ are assumed independent. Consider now a finite measure γ supported on $\mathbb{N}^*$, and for $y \in \bar{\mathbb{N}}^* = \mathbb{N}^* \cup \{\infty\}$ let

$$\Gamma(t) = \Gamma^y(t) = \gamma_y\, T_0 + \sum_{x=1}^{\infty} \gamma_x \sum_{i=1}^{N_t^{(x)}} T_i^{(x)}, \tag{2}$$

where, by convention, $\sum_{i=1}^{0} T_i^{(x)} = 0$ for every x, and $\gamma_\infty = 0$. We define the process Y on $\bar{\mathbb{N}}^*$ starting at $y \in \bar{\mathbb{N}}^*$ as follows. For $t \geq 0$

$$Y_t = \begin{cases} y, & \text{if } 0 \leq t < \gamma(y) T_0, \\ x, & \text{if } \Gamma(\sigma_j^{(x)}-) \leq t < \Gamma(\sigma_j^{(x)}) \text{ for some } 1 \leq j < \infty, \\ \infty, & \text{otherwise.} \end{cases} \tag{3}$$

This process, which we here call the K process with parameter γ, was introduced and studied in [10], where it was shown to arise as limits of trap models in the complete graph with n vertices as $n \to \infty$ (see Lemma 3.11 in [10]). In the next section, we derive a similar result for the hypercube. See Theorem 1. This is our main technical result. Then, in the following section, we apply that result to get the scaling limits of the REM-like trap model and the Random Hopping Times dynamics for the REM in ergodic time scales as K processes. See Sect. 3.

2 Convergence to the K Process

Theorem 1. *Suppose that, as $d \to \infty$, $\tilde{\gamma}^d$ converges weakly to a finite measure $\tilde{\gamma}$ supported on $\mathbb{N}^*$, and that X_0^d converges weakly to a probability measure μ on $\bar{\mathbb{N}}^*$. Then, X^d converges weakly in Skorohod space as $d \to \infty$ to a K process with parameter $\tilde{\gamma}$ and initial measure μ.*

This result extends the analysis performed in [10] for the trap model in the complete graph, with a similar approach (see Lemma 3.11 in [10] and its proof). The extra difficulty here comes from the fact that the transition probabilities in the hypercube are not uniform in the state space, as is the case in the complete graph. However, all that is indeed needed is an approximate uniform entrance law in finite sets of states. This result, a key tool used several times below, is available from [3]. We state it next, in a form suitable to our purposes, but first some notation. Let $\mathscr{X}$ denote the embedded chain of X^d and for a given fixed finite subset $\mathscr{J}$ of $\mathbb{N}^*$, let $\mathscr{T}_{\mathscr{J}}$ denote the entrance time of $\mathscr{X}$ in $\mathscr{J}$, namely,

$$\mathscr{T}_{\mathscr{J}} = \inf\{n \geq 0 : \mathscr{X}_n \in \mathscr{J}\}. \tag{4}$$

Proposition 2 (Corollary 1.5 [3]).

$$\lim_{d\to\infty} \max_{x\notin\mathscr{J}, y\in\mathscr{J}} \left| \mathbb{P}(\mathscr{X}_{\mathscr{T}_{\mathscr{J}}} = y | \mathscr{X}_0 = x) - \frac{1}{|\mathscr{J}|} \right| = 0. \tag{5}$$

Here $|\cdot|$ denotes cardinality.

Remark 3. Corollary 1.5 of [3] is actually more precise and stronger than the above statement, with error of approximation estimates, and holding for $\mathscr{J}$ depending on d in a certain manner as well.

Remark 4. Equation (5) is the only fact about the hypercube used in the proof of Theorem 1. This result would thus hold as well for other graphs with the same property. The hypercube has nevertheless been singled out in analyses of dynamics of mean field spin glasses (see above mentioned references), and that is a reason for us to do the same here.

2.1 Proof of Theorem 1

The strategy is to approximate X^d for d large by a trap model in the complete graph with vertex set $\mathscr{M} = \{1, \dots, M\}$ and mean waiting times $\{\tilde{\gamma}_1, \dots, \tilde{\gamma}_M\}$ for $M \leq d$ large. Let Y^M denote the latter process, and let us put $Y_0^M = Y_0 \, 1\{Y_0 \in \mathscr{M}\} + W \, 1\{Y_0 \notin \mathscr{M}\}$, with W an independent uniform random variable in $\mathscr{M}$. To accomplish the approximation, we will resort to an intermediate process, which we next describe. We start by considering $\hat{X}^d$, the trap model on $\mathscr{D}$ obtained from X^d by replacing its set of mean waiting times (see (1) above) by $\{\tilde{\gamma}_x, \, x \in \mathscr{D}\}$. The intermediate process we will consider is then $\hat{X}^d$ *restricted* to $\mathscr{M}$, denoted $\hat{X}^{d,M}$: this is the Markov process obtained from $\hat{X}^d$ by observing it only when it is in $\mathscr{M}$ (with time stopping for $\hat{X}^{d,M}$ when $\hat{X}^d$ is outside $\mathscr{M}$).

The approximations will be strong ones: we will couple X^d to $\hat{X}^{d,M}$ and $\hat{X}^{d,M}$ to Y^M, in the spirit of Theorem 5.2 in [10], where the approximation of Y by Y^M, needed here as the last step of the argument, was established. In particular, we also couple X_0^d to Y_0 so that the former converges almost surely to the latter as $d \to \infty$.

2.1.1 Coupling of $\hat{X}^{d,M}$ and Y^M

We first look at the embedded chains of $\hat{X}^{d,M}$ and Y^M. Let $(p_{ij}^{d,M})_{i,j \in \mathscr{M}}$ be the transition probabilities of the former chain, and let $\hat{p} = \min_{i,j \in \mathscr{M}} p_{ij}^{d,M}$. We leave it to the reader to check that there is a coupling between both chains which agrees at each step with probability at least $M\hat{p}$. We resort to such a coupling. Proposition 2 implies that

$$M\hat{p} \to 1 \tag{6}$$

as $d \to \infty$ for every M fixed.

Since $\hat{X}^{d,M}$ and Y^M have the same mean waiting times at each site, we can couple them in such a way that they have the same waiting times at successive visits to each site. One may also find a coupling of $\hat{X}_0^{d,M}$ and Y_0^M such that

$$\mathbb{P}(\hat{X}_0^{d,M} \neq Y_0^M) \to 0 \tag{7}$$

as $d \to \infty$. Resorting also to that coupling, we get the following result.

Lemma 5. *For every T and M fixed, we have*

$$\mathbb{P}(\hat{X}_t^{d,M} = Y_t^M, \; t \in [0, T]) \to 1 \tag{8}$$

as $d \to \infty$.

Proof. Let N_T denote the number of jumps of Y^M in the time interval $[0, T]$, and $0 = t_0, t_1, \dots, t_{N_T}$ the respective jump times. We conclude from the above discussion that

$$\mathbb{P}(\hat{X}_t^{d,M} = Y_t^M, t \in [0,T] | N_T = k) = \mathbb{P}(\hat{X}_{t_i}^{d,M} = Y_{t_i}^M, i = 0,1,\ldots,k | N_T = k)$$
$$\geq \mathbb{P}(\hat{X}_0^{d,M} = Y_0^M)\,(M\hat{p})^k, \tag{9}$$

and the result follows from (6), (7) and dominated convergence (since $M\hat{p}$ is bounded above by 1 for all d and M). □

2.1.2 Coupling of X^d and $\hat{X}^{d,M}$

We couple X^d and $\hat{X}^d$ (the latter process was defined at the beginning of the section) in the following way. Note that $\mathscr{X}$ is their common embedded chain. We then make the successive sojourn times of X^d and $\hat{X}^d$, starting from the first ones, be given by $\tilde{\gamma}^d_{\mathscr{X}_0} T_0^{\mathscr{X}_0}, \tilde{\gamma}^d_{\mathscr{X}_1} T_1^{\mathscr{X}_1}, \ldots$ and $\tilde{\gamma}_{\mathscr{X}_0} T_0^{\mathscr{X}_0}, \tilde{\gamma}_{\mathscr{X}_1} T_1^{\mathscr{X}_1}, \ldots$, respectively, where the common $T_0^x, T_1^x, \ldots, x \in \mathbb{N}^*$, are i.i.d. rate 1 exponential random variables.

With a view towards approximating X^d and $\hat{X}^{d,M}$ strongly in Skorohod space, we introduce a *time distortion function* useful for that (see (11) below). For K a fixed positive integer, let $\mathscr{K}$ denote the set $\{1,\ldots,K\}$, and consider the successive entrance and exit times of X^d and $\hat{X}^{d,M}$ in and out of $\mathscr{K}$ defined as follows. Let $\tau_0 = \tau_0^* = \xi_0 = \xi_0^* = 0$ and for $i \geq 1$, let

$$\tau_i = \inf\{t \geq \tau_{i-1}^* : \hat{X}_t^{d,M} \in \mathscr{K}\}, \qquad \tau_i^* = \inf\{t \geq \tau_i : \hat{X}_t^{d,M} \notin \mathscr{K}\}, \tag{10}$$

and similarly define ξ_i and ξ_i^*, $i \geq 1$ with X^d replacing $\hat{X}^{d,M}$. See Fig. 1 below.

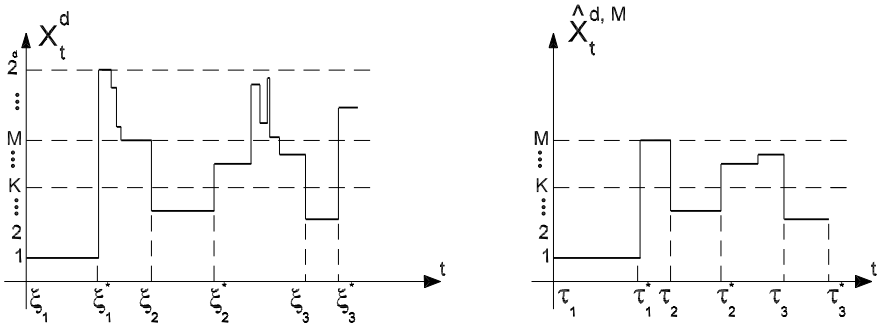

Fig. 1 Trajectories of X^d and $\hat{X}^{d,M}$

Now for $T > 0$ fixed, let $N = \min\{i \geq 1 : \tau_i > T\}$ and define

$$\tilde{\lambda}_t = \begin{cases} \xi_j + \frac{\xi_j^* - \xi_j}{\tau_j^* - \tau_j}(t - \tau_j), & \text{if } \tau_j < t \leq \tau_j^* \text{ for some } 0 \leq j < N, \\ \xi_j^* + \frac{\xi_{j+1} - \xi_j^*}{\tau_{j+1} - \tau_j^*}(t - \tau_j^*), & \text{if } \tau_j^* < t \leq \tau_{j+1} \text{ for some } 0 \leq j < N, \\ \xi_N + (t - \tau_N), & \text{if } t \geq \tau_N. \end{cases} \tag{11}$$

Here and below, we interpret $0/0$ as 1. See Fig. 2 below.

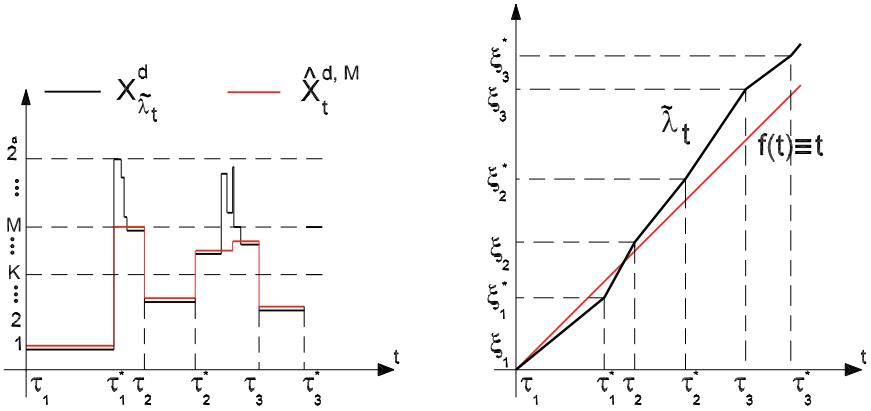

Fig. 2 Superimposed trajectories of X^d with time distorted by $\tilde{\lambda}$ and $\hat{X}^{d,M}$ (left), and superposition of the graphs of $\tilde{\lambda}$ and the identity (right)

Remark 6. With the above definition of $\tilde{\lambda}$, we first note that $\hat{X}^{d,M}_t = X^d_{\tilde{\lambda}_t}$ whenever any of both processes is visiting $\mathscr{K}$ before time τ_N.

As part of the norm in Skorohod space, we consider the class Λ of nondecreasing Lipschitz functions mapped from $[0, \infty)$ onto $[0, \infty)$, and the following function on Λ

$$\phi(\lambda) = \sup_{0 \le s < t} \left| \log \frac{\lambda_t - \lambda_s}{t - s} \right|. \tag{12}$$

We have from (11) above that

$$\phi(\tilde{\lambda}) \le \max_{1 \le j \le N} \left| \log \frac{\xi_j - \xi^*_{j-1}}{\tau_j - \tau^*_{j-1}} \right| \vee \max_{1 \le j \le N} \left| \log \frac{\xi^*_j - \xi_j}{\tau^*_j - \tau_j} \right|. \tag{13}$$

Below, we will consider the events A_j, $j \ge 0$, as follows.

$$A_0 = \{X^d_0 \in \mathscr{K}\} \cup \{\text{there exists } 0 \le t < \xi_1 \text{ such that } X^d_t \in \mathscr{M} \setminus \mathscr{K}\}, \tag{14}$$

$$A_j = \{\text{there exists } \xi^*_j \le t < \xi_{j+1} \text{ such that } X^d_t \in \mathscr{M} \setminus \mathscr{K}\}, \ j \ge 1. \tag{15}$$

It follows from Proposition 2 that for $j \ge 0$

$$\lim_{d \to \infty} \inf_{x \notin \mathscr{M}} \mathbb{P}(A_j | X^d_{\xi^*_j} = x) = 1 - K/M. \tag{16}$$

Notice that the probability on the left hand side of (16) does not depend on j; we thus get that

$$\lim_{M \to \infty} \lim_{d \to \infty} \mathbb{P}(A_j) = 1 \quad \text{uniformly on } j \ge 0. \tag{17}$$

2.1.3 Conclusion of proof of Theorem 1

Let $D_{\bar{\mathbb{N}}^*}([0,\infty))$ be the (Skorohod) space of cádlág functions of $[0,\infty)$ to $\bar{\mathbb{N}}^*$ with metric

$$\rho(f,g) := \inf_{\lambda\in\Lambda}\left[\phi(\lambda) \vee \int_0^\infty e^{-u}\rho(f,g,\lambda,u)du\right], \tag{18}$$

where

$$\rho(f,g,\lambda,u) := \sup_{t\geq 0}\left|[f(t\wedge u)]^{-1} - [g(\lambda(t)\wedge u)]^{-1}\right|; \tag{19}$$

see Sect. 3.5 in [9]; Λ and ϕ were defined in the paragraph of (12) above, and $\infty^{-1} = 0$.

It follows from Lemma 3.11 in [10] that Y^M converges weakly to Y in Skorohod space as $M \to \infty$. In order to prove Theorem 1, it thus suffices to show the following result.

Lemma 7. *With the above construction of X^d and Y^M, we have that for every $\epsilon > 0$*

$$\lim_{M\to\infty}\limsup_{d\to\infty}\mathbb{P}(\rho(X^d, Y^M) > \epsilon) = 0. \tag{20}$$

Proof. Given $\epsilon > 0$, let $T_\epsilon = -\log(\epsilon/2)$. Then choosing λ to be the identity, noticing that ρ in (19) is bounded above by 1, and using Lemma 5, we find that for every $M > 0$

$$\mathbb{P}(\rho(\hat{X}^{d,M}, Y^M) > \epsilon/2) \leq \mathbb{P}(\hat{X}_t^{d,M} \neq Y_t^M \text{ for some } t \in [0, T_\epsilon]) \to 0 \tag{21}$$

as $d \to \infty$. So, to establish Lemma 7, it suffices to prove Lemma 8 below. □

Lemma 8. *With above construction of X^d and $\hat{X}^{d,M}$, we have that for every $\epsilon > 0$*

$$\lim_{M\to\infty}\limsup_{d\to\infty}\mathbb{P}(\rho(\hat{X}^{d,M}, X^d) > \epsilon) = 0. \tag{22}$$

Proof. Let $T = T_\epsilon = -\log\epsilon$, choose K such that $|x^{-1} - y^{-1}| \leq \epsilon$ for every $x, y \in \bar{\mathbb{N}}^* \setminus \mathscr{K}$, and consider $\tilde{\lambda}$ as in (11) with such T and K. Then, by Remark 6 and (12), we see that it suffices to show that for every $\epsilon > 0$

$$\lim_{M\to\infty}\limsup_{d\to\infty}\mathbb{P}\left(\max_{1\leq j\leq N}\left|\log\frac{\xi_j^* - \xi_j}{\tau_j^* - \tau_j}\right| > \epsilon\right) = 0, \tag{23}$$

and

$$\lim_{M\to\infty}\limsup_{d\to\infty}\mathbb{P}\left(\max_{1\leq j\leq N}\left|\log\frac{\xi_j - \xi_{j-1}^*}{\tau_j - \tau_{j-1}^*}\right| > \epsilon\right) = 0. \tag{24}$$

□

Proof of (23). One readily checks that

$$\max_{1\le j\le N}\left|\log\frac{\xi_j^*-\xi_j}{\tau_j^*-\tau_j}\right|\le\max_{x\in\mathscr{K}}\left|\log\frac{\tilde\gamma_x^d}{\tilde\gamma_x}\right|, \tag{25}$$

and (23) follows immediately from the assumption that $\tilde\gamma^d\to\tilde\gamma$ as $d\to\infty$. □

Proof of (24). Let $\tilde\gamma^{d,K}=\{\tilde\gamma_x^{d,K}:=\tilde\gamma_x^d\wedge\tilde\gamma_K^d, x\in\mathscr{D}\}$, and consider the trap model $X^{d,K}$ with mean waiting times $\tilde\gamma^{d,K}$ coupled to X^d so that both processes have the same embedded chain $\mathscr{X}$ and the respective sojourn times are given by $\tilde\gamma^{d,K}_{\mathscr{X}_0}T_0^{\mathscr{X}_0},\tilde\gamma^{d,K}_{\mathscr{X}_1}T_1^{\mathscr{X}_1},\dots$ and $\tilde\gamma^{d}_{\mathscr{X}_0}T_0^{\mathscr{X}_0},\tilde\gamma^{d}_{\mathscr{X}_1}T_1^{\mathscr{X}_1},\dots$

Let now $\tilde X^{d,K}$ denote the process $X^{d,K}$ restricted to $\mathscr{K}$ (analogously as $\hat X^{d,M}$), with $\tilde{\mathscr{X}}$ its embedded chain. Let N^K denote the number of jumps of $\tilde X^{d,K}$ up to time T. Notice that N^K is a Poisson process with rate $1/\tilde\gamma_K^d$ independent of $\mathscr{X}$ and of the history of X^d in the time intervals $[\xi_j^*,\xi_{j+1})$, $j\ge0$. Thus, the probability on the left hand side of (24) is bounded above by

$$\mathbb{P}\left(\max_{1\le j\le N^K}\left|\log\frac{U_j}{V_j}\right|>\epsilon\right)\le\sum_{n=1}^{\infty}\sum_{j=1}^{n}\mathbb{P}\left(\left|\log\frac{U_j}{V_j}\right|>\epsilon\right)\mathbb{P}(N^K=n), \tag{26}$$

where $U_j:=\xi_j-\xi_{j-1}^*$ and $V_j:=\tau_j-\tau_{j-1}^*$. We now estimate the first probability on the right hand side of (26). We first note that from (17), and the fact that $\mathbb{E}(N^K)$ is finite and independent of d, M, we may insert A_j in that probability. We next write $U_j=W_j+R_j$, where R_j is the time spent by X^d in $\mathscr{D}\setminus\mathscr{M}$ during the time interval $[\xi_{j-1}^*,\xi_j)$. From the elementary inequality $|\log(x+y)|\le|\log x|+y$, valid for all $x, y>0$, we get that

$$\mathbb{P}\left(\left|\log\frac{U_j}{V_j}\right|>\epsilon,\ A_j\right)\le\mathbb{P}\left(\left|\log\frac{W_j}{V_j}\right|>\epsilon/2,\ A_j\right)+\mathbb{P}\left(R_j>\epsilon V_j/2\right). \tag{27}$$

Arguing as in (25) above, we find that the first event in the first probability on the right hand side of (27) is empty as soon as $\max_{x\in\mathscr{M}}|\log\frac{\tilde\gamma_x^d}{\tilde\gamma_x}|\le\epsilon/2$, thus from $\tilde\gamma^d\to\tilde\gamma$ as $d\to\infty$ we only need to consider the second probability on the right hand side of (27). One readily checks that it is bounded above by

$$\max_{x\notin\mathscr{K}}\mathbb{P}\big(R_j>\epsilon V_j/2\big|X^d_{\xi_{j-1}^*}=x\big) \tag{28}$$

for all $j\ge0$, and that the above expression does not depend on j. It is enough then to show that for any $\epsilon>0$

$$\mathbb{P}\big(R_1>\epsilon V_1|X_0^d=x\big)=:\mathbb{P}_x(R_1>\epsilon V_1)\to0 \tag{29}$$

as $d\to\infty$ and then $M\to\infty$, uniformly in $x>K$. This is readily seen to follow from the facts that

$$\lim_{M\to\infty}\limsup_{d\to\infty}\max_{x\notin\mathscr{K}}\mathbb{P}_x(R_1>\epsilon)=0 \tag{30}$$

for any $\epsilon > 0$, and that, given $\delta > 0$, there exists $\epsilon > 0$ such that

$$\limsup_{M\to\infty} \limsup_{d\to\infty} \max_{x\notin\mathscr{K}} \mathbb{P}_x(V_1 \le \epsilon) \le \delta. \tag{31}$$

□

Proof of (30). Let $x \notin \mathscr{K}$ be arbitrary. We will estimate

$$\mathbb{E}_x(R_1) := \mathbb{E}(R_1 | X_0^d = x) = \sum_{y=M+1}^{d} \tilde{\gamma}_y^d \, \mathbb{E}_x(\mathscr{L}(y)), \tag{32}$$

where $\mathscr{L}(y)$ is the number of visits of $\mathscr{X}$ to y from time 0 till its first entrance in $\mathscr{K}$.

Let $\mathscr{K}_y = \mathscr{K} \cup \{y\}$ and consider the discrete time Markov process $\bar{\mathscr{X}}$ such that $\bar{\mathscr{X}}_0 = x$ and otherwise $\bar{\mathscr{X}}$ is the restriction of $\mathscr{X}$ to $\mathscr{K}_y = \mathscr{K} \cup \{y\}$, and let $\bar{\mathscr{L}}(y)$ denote the number of visits of $\bar{\mathscr{X}}$ to y from time 0 till its first entrance in $\mathscr{K}$. Clearly,

$$\mathscr{L}(y) = \bar{\mathscr{L}}(y). \tag{33}$$

Now let $\mathscr{X}^*$ denote the Markov chain on $\mathscr{K}_y \cup \{x\}$ with the following set of transition probabilities. Let $p^1 = (p^1_{wz},\ w, z \in \mathscr{K}_y \cup \{x\})$, and $p^2 = (p^2_{wz},\ w, z \in \mathscr{K}_y \cup \{x\})$ denote the sets of transition probabilities of $\bar{\mathscr{X}}$ and $\mathscr{X}^*$, respectively. We make

$$p^2_{xy} = p^2_{yy} = p^* := \max\{p^1_{wz};\ w = x, y;\ z \in \mathscr{K}_y\}, \tag{34}$$

and the remaining p^2_{wz} can be assigned arbitrarily with the only obvious condition that p^2 is a set of transition probabilities on $\mathscr{K}_y$. Let $\mathscr{L}^*(y)$ denote the number of visits of $\mathscr{X}^*$ to y from time 0 till its first entrance in $\mathscr{K}$. One readily checks that $\mathscr{L}^*(y)$ is a Geometric random variable with parameter $1 - p^*$ and that it stochastically dominates $\bar{\mathscr{L}}(y)$. From this and (33), we conclude that

$$\mathbb{E}_x(\mathscr{L}(y)) \le \frac{p^*}{1 - p^*} \tag{35}$$

uniformly in $x \notin \mathscr{K}$. Proposition 2 then implies that

$$\limsup_{d\to\infty} \max_{x\notin\mathscr{K}} \mathbb{E}_x(\mathscr{L}(y)) \le \frac{1}{K}. \tag{36}$$

It follows readily from this, (32) and the assumption that $\tilde{\gamma}^d \to \tilde{\gamma}$ as $d \to \infty$ that

$$\limsup_{d\to\infty} \max_{x\notin\mathscr{K}} \mathbb{E}_x(R_1) \le \frac{1}{K} \sum_{y=M+1}^{\infty} \tilde{\gamma}_y, \tag{37}$$

and (30) follows (using Markov's inequality), since $\tilde{\gamma}$ is a finite measure on $\mathbb{N}^*$. □

Proof of (31). Let us fix $x_0 \notin \mathscr{K}$. Consider the Markov process $Z = (Z_t)_{t\geq 0}$ on $\mathscr{M}$ such that $Z_0 = x_0$, for every $x \in \mathscr{M}$ the waiting time at x before jumping is exponential with mean $\tilde{\gamma}_x$, and the transition probability to $y \in \mathscr{M}$ equals $\hat{p}$, if $y \notin \mathscr{K}$, and $\frac{1-(M-K)\hat{p}}{K}$, if $y \in \mathscr{K}$, where $\hat{p}$ was defined in the paragraph of (6) above.

One readily checks that, given $X_0^d = x_0$, V_1 stochastically dominates S, the time Z spends in $\mathscr{M} \setminus \mathscr{K}$ before hitting $\mathscr{K}$ for the first time. Since $\tilde{\gamma}_x$ is decreasing in x, by the construction of Z, we have that, for every $L \in \{K+1, \ldots, M\}$, S dominates stochastically the random variable $\tilde{\gamma}_L T 1_C$, where C is the event that Z visits $\{K+1, \ldots, L\}$ before hitting $\mathscr{K}$ for the first time, T is an exponential random variable of rate 1, and $1_\cdot$ is the usual indicator function.

Let now $\mathscr{Z}$ denote the embedded chain for Z, and $\mathscr{T}_L = \inf\{n \geq 1 : \mathscr{Z}_n \in \{1, \ldots, L\}\}$. Then

$$\begin{aligned}
&\mathbb{P}(C|\mathscr{Z}_0 = x_0) \\
&\quad = \mathbb{P}(\mathscr{Z}_{\mathscr{T}_L} \in \{K+1, \ldots, L\} | \mathscr{Z}_{\mathscr{T}_L} \leq L, \mathscr{Z}_0 = x_0) \\
&\quad = \frac{(L-K)\hat{p}}{K[\frac{1-(M-K)\hat{p}}{K}] + (L-K)\hat{p}} = \frac{(L-K)\hat{p}}{1-(M-L)\hat{p}} \\
&\quad = \frac{(L-K)M\hat{p}}{(1-M\hat{p})M + LM\hat{p}} \to \frac{(L-K)}{L} = 1 - \frac{K}{L}
\end{aligned} \tag{38}$$

as $d \to \infty$ uniformly in x_0; see (6).

We conclude that

$$\limsup_{M\to\infty} \limsup_{d\to\infty} \max_{x\notin\mathscr{K}} \mathbb{P}_x(V_1 \leq \epsilon) \leq \mathbb{P}(\tilde{\gamma}_L T \leq \epsilon) + \frac{K}{L} \tag{39}$$

for every $K < L$. Thus, given K and $\delta > 0$, we first choose L such that $\frac{K}{L} \leq \delta/2$, and then $\epsilon > 0$ such that $\mathbb{P}(\tilde{\gamma}_L T \leq \epsilon) \leq \delta/2$, and we are done. □

3 The REM-Like Trap Model and the Random Hopping Times Dynamics for the REM

In this section we apply Theorem 1 to obtain the scaling limits of two disordered trap models in the hypercube, namely trap models in the hypercube whose mean waiting times are random variables.

3.1 The REM-Like Trap Model

Let $\tau^d := \{\tau_v^d,\ v \in \mathscr{V}\}$, an i.i.d. family of random variables in the domain of attraction of an α-stable law with $0 < \alpha < 1$, be the mean waiting times of a trap

model in $\mathscr{H}$. Let us then consider as before $\tilde{\tau}^d := \{\tilde{\tau}^d_x,\ x \in \mathscr{D}\}$, the decreasing order statistics of τ (with an arbitrary tie breaking rule), and let Y^d be the mapped process on $\mathscr{D}$.

Now let c_d be a scaling factor such that $\hat{\tau}^d := c_d\,\tilde{\tau}^d$ converges to the increments in $[0, 1]$ of an α-stable subordinator. Namely,

$$c_d = \left(\inf\{t \geq 0 : \mathbb{P}(\tau_0 > t) \leq 2^{-d}\}\right)^{-1}. \tag{40}$$

Let us now consider Y^d speeded up by c_d^{-1}, namely $\hat{Y}^d_t = Y^d(t/c_d)$, $t \geq 0$. Notice that $\hat{Y}^d$ is a trap model on $\mathscr{H}$ with mean waiting times given by $\hat{\tau}^d$.

Let $\hat{\gamma} = \{\hat{\gamma}_i,\ i \in \mathbb{N}^*\}$ denote the increments in $[0, 1]$ of an α-stable subordinator in decreasing order.

Corollary 9. *Suppose that $\hat{Y}^d_0$ converges weakly to a probability measure μ on $\bar{\mathbb{N}}^*$. Then*

$$(\hat{Y}^d, \hat{\tau}^d) \Rightarrow (Y, \hat{\gamma}), \tag{41}$$

where Y is a K process with parameter $\hat{\gamma}$ and initial measure μ, and $\Rightarrow$ means weak convergence in the product of Skorohod norm and weak convergence norm in the space of finite measures in $\mathbb{N}^*$.

Remark 10. In [10], a similar result was proved for the REM-like trap model in the complete graph. See Theorem 5.2 in that reference.

Proof of Corollary 9. We can suppose that we are in a probability space where $\hat{\tau}^d \to \hat{\gamma}$ almost surely (see proof of Theorem 5.2 in [10] for an explicit argument). We can then invoke Theorem 1 to get that $\hat{Y}^d \Rightarrow Y$, and the full result follows. □

3.2 Random Hopping Times Dynamics for the REM

This is a dynamics whose equilibrium is the Random Energy Model. Let $H^d := \{H^d_v,\ v \in \mathscr{V}\}$ be an i.i.d. family of standard normal random variables, and make $\tau^d := \{\tau^d_v,\ v \in \mathscr{V}\}$, where $\tau^d_v = e^{\beta\sqrt{d}H^d_v}$. Defining now $\tilde{\tau}^d$, $\hat{\tau}^d$, Y^d and $\hat{Y}^d$ as above, with

$$c_d = e^{-\frac{2\log 2}{\alpha}d + \frac{1}{2\alpha}\log d}, \tag{42}$$

with $\alpha = \sqrt{2\log 2}/\beta$, we have that, if $\alpha < 1$, then Corollary 9 holds in this case as well, with $\hat{\gamma}$ and μ as before.

The proof starts from the known result that in this case $\hat{\tau}^d \Rightarrow \hat{\gamma}$ (see Remark to Theorem 2 in [12]). Again, as in the proof of Corollary 9 above, we can go to a probability space where the latter convergence is almost sure, and close the argument in the same way.

Remark 11. The time scale $t \to t/c_d$ adopted in the above models is the *ergodic* time scale mentioned in [8]. Under shorter scalings (i.e., $t \to t/c'_d$, with $c'_d \gg c_d$)

the model exhibits *aging* (when starting from the uniform distribution), and under longer ones ($c'_d \ll c_d$), the model reaches equilibrium. More precisely, under shorter scalings, we have that as $d \to \infty$

$$\mathbb{P}_{\mu^d}\left(Y^d(t/c'_d) = Y^d((t+s)/c'_d)\right) \to \mathscr{R}(s/t), \tag{43}$$

where μ^d is the initial uniform distribution on $\mathscr{D}$, and $\mathscr{R}$ is a nontrivial function such that $\mathscr{R}(0) = 1$ and $\lim_{x\to\infty} \mathscr{R}(x) = 0$. Indeed, for the models of this section (as well as in many other instances in the references), $\mathscr{R}$ is the arcsine law:

$$\mathscr{R}(x) = \frac{\sin(\pi\alpha)}{\pi} \int_{\frac{x}{1+x}}^{1} s^{-\alpha}(1-s)^{\alpha-1}\, ds. \tag{44}$$

See [1]. Under longer scalings, it can be shown that $Y^d(t/c'_d) \Rightarrow \bar{\gamma}$ as $d \to \infty$ for every $t > 0$, where $\bar{\gamma}$ is $\hat{\gamma}$ normalized to be a probability measure. It is the limiting equilibrium measure, or more precisely, the equilibrium measure of Y.

Remark 12. It can be shown that Y exhibits aging at a vanishing time scale (when starting from ∞), i.e.

$$\mathbb{P}_{\infty}\left(Y(\epsilon t) = Y(\epsilon(t+s))\right) \to \mathscr{R}(s/t) \tag{45}$$

as $\epsilon \to 0$. See Theorem 5.11 in [10]. This is in agreement with (43).

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Spontaneous Replica Symmetry Breaking in the Mean Field Spin Glass Model

Francesco Guerra

Abstract We give a short review about recent results in the study of the mean field Sherrington-Kirkpatrick model for a spin glass. Our methods are essentially based on interpolation and comparison arguments for families of Gaussian random variables. In particular we show how to control the infinite volume limit for the free energy density, and how to relate the model to its replica symmetric approximation. We discuss also the mechanism of replica symmetry breaking, by using suitable interpolation methods. Our results are in agreement with those obtained in the frame of the replica trick through the Parisi Ansatz. Finally, we point out some possible further developments of the theory.

1 Introduction

More than thirty years ago, David Sherrington and Scott Kirkpatrick introduced a celebrated mean field model for spin glasses [27, 18], then considered to be a "solvable model".

It is hard to overestimate the impact of this model on the theoretical physics research. During the three decades after its introduction, hundreds and hundreds of papers have been devoted to the study of its properties, even through numerical methods.

The relevance of the model surely comes from the fact that it is able to represent successfully, at least at the level of the mean field approximation, some important features of the physical spin glass systems, of great interest for their peculiar properties.

Let us recall that some dilute magnetic alloys, called spin glasses, are extremely interesting systems from a physical point of view. Their peculiar feature is to exhibit

Francesco Guerra
Department of Physics, Sapienza University of Rome and INFN, Section of Roma 1, Rome, Italy,
e-mail: francesco.guerra@roma1.infn.it

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a new magnetic phase, where magnetic moments are frozen into disordered equilibrium orientations, without any long-range order. We refer for example to [33] and [29] for general reviews about the physical properties of spin glasses. The experimental laboratory investigation about concrete spin glasses is a very difficult subject, because of their peculiar properties. In particular, these materials have some very slowly relaxing modes, with consequent memory effects. Therefore, even the very basic physical concept of a system at thermodynamical equilibrium, at a given temperature, meets a difficult empirical realization.

From a theoretical point of view, some models have been proposed, attempting to capture the essential physical features of spin glasses, in the frame of very simple assumptions.

The basic model has been proposed by Edwards and Anderson [5] many years ago. It is a simple extension of the well-known nearest neighbour Ising model for ferromagnetism to the spin glass case. Consider a large region Λ of the unit lattice in d dimensions. Let us associate an Ising spin $\sigma(n)$ to each lattice site n. Then, we introduce the lattice Edwards-Anderson Hamiltonian

$$H_\Lambda(\sigma, J) = -\sum_{(n,n')} J(n, n')\sigma(n)\sigma(n').$$

Here, the sum runs over all couples of nearest neighbour sites in Λ, and J are quenched random couplings, assumed for simplicity to be independent identically distributed random variables, with centered unit Gaussian distribution. The quenched character of the J means that they do not participate in the thermodynamic equilibrium, but act as a kind of random external noise on the coupling of the σ variables. In the expression of the Hamiltonian, we have indicated with σ the set of all $\sigma(n)$, and with J the set of all $J(n, n')$. The region Λ must be taken very large, letting it invade the whole lattice in the limit. The physical motivation for this choice is that for real spin glasses, due to quantum interference effects, the effective interaction between the ferromagnetic domains dissolved in the matrix of the alloy oscillates in sign according to distance. This feature is taken into account in the model through the random character of the couplings between spins.

Even though very drastic simplifications have been introduced in the formulation of this model, as compared to the extremely more complicated nature of physical spin glasses, nevertheless a rigorous study of all properties emerging from the static and dynamic behavior of a thermodynamic system of this kind is far from being complete. In particular, with reference to static equilibrium properties, it is not possible yet to reach a completely substantiated description of the phases emerging in the low temperature region. Even by relying on physical intuition, we get completely different answers from different people working in the field.

It is very well known that a mean-field version can be associated to the ordinary ferromagnetic Ising model (see for example [28]). The same is possible for the disordered model described by the Edwards-Anderson Hamiltonian defined above. Now we consider a number of sites $i = 1, 2, \ldots, N$, not organized in a lattice, and

let each spin $\sigma(i)$ at site i interact with all other spins, in the presence of a quenched noise J_{ij}. The precise form of the Hamiltonian will be given in Sect. 2.

This is the mean field model for spin glasses, introduced by David Sherrington and Scott Kirkpatrick.

There is also an additional very important reason for the relevance of this model, and related ones. In fact, recently it has become progressively clear that disordered systems of the Sherrington-Kirkpatrick type, and their generalizations, seem to play a very important role for theoretical and practical applications to hard optimization problems, as it is shown for example by Marc Mézard, Giorgio Parisi and Riccardo Zecchina in [22].

It is interesting to remark that the original paper was entitled "Solvable Model of a Spin-Glass", while a previous draft, according to what recalled by David Sherrington, contained even the stronger denomination "Exactly Solvable". However, it turned out that the very natural solution devised by the authors is valid only at high temperatures, or for large external magnetic fields. At low temperatures, the proposed solution exhibits a nonphysical drawback given by a negative entropy, as properly recognized by the authors in their very first paper.

It took a few years to find an acceptable solution. This was done by Giorgio Parisi in a series of papers, by marking a radical departure from the previous methods. In fact, a very deep method of "spontaneous replica symmetry breaking" was developed. As a consequence the physical content of the theory was encoded in a functional order parameter of new type, and a remarkable structure began to show up for the pure states of the theory, characterized by a kind of hierarchical, ultrametric organization. These very interesting developments, due to Giorgio Parisi, and his coworkers, are explained in a challenging way in the classical book [20]. Part of this structure will be recalled in the following.

It is important to remark that the Parisi solution is presented in the form of an ingenious and clever *Ansatz*. Until a few years ago it was not known whether this *Ansatz* would give the true solution for the model, in the so-called thermodynamic limit, when the size of the system becomes infinite, or it would be only a very good approximation to the true solution.

The general structures offered by the Parisi solution, and their possible generalizations for similar models, exhibit an extremely rich and interesting mathematical content. In a very significant way, Michel Talagrand inserted a strongly suggestive sentence in the title to his recent book [31]: "Spin glasses: a challenge for mathematicians".

As a matter of fact, the problem of giving a proper mathematical understanding of the spin glass structure is extremely difficult. In this talk, we would like to recall the main features of a very powerful method, yet extremely simple in its very essence, based on comparison and interpolation arguments on families of Gaussian random variables.

The method found its first simple application in [10], where it was shown that the Sherrington-Kirkpatrick replica symmetric approximate solution is a rigorous lower bound for the quenched free energy of the system, uniformly in the size, for any value of the temperature and the external magnetic field. Then, it was possible

to reach a long awaited result [15]: the convergence of the free energy density in the thermodynamic limit, by an intermediate step where the quenched free energy was shown to be subadditive in the size of the system.

Moreover, still by a generalized interpolation on families of Gaussian random variables, the first mentioned result, on the replica symmetric solution, was extended to give a rigorous proof that the expression given by the Parisi *Ansatz* is also a lower bound for the quenched free energy of the system, uniformly in the size [12]. The method gives not only the bound, but also the explicit form of the correction terms in the form of a sum rule. As a recent and very important result, Michel Talagrand has been able to dominate these correction terms, showing that they vanish in the thermodynamic limit. This extraordinary achievement was firstly announced in a short note [30], containing only a synthetic sketch of the proof, and then presented with all details in a long paper in Annals of Mathematics [32].

The interpolation method is also at the basis of the far-reaching generalized variational principle proven by Michael Aizenman, Robert Sims and Shannon Starr in [1].

In this lecture, we will concentrate mostly on the main questions connected with the free energy. In particular, we will consider the subadditivity with respect to the system size, the existence of the infinite-volume limit, the broken replica symmetry sum rules and bounds, and the Parisi variational principle. Our treatment will be as simple as possible, by relying on the basic structural properties, and by describing methods of presumably very long lasting power.

The organization of the paper is as follows. In Sect. 2 we explain the basic features of the mean field spin glass models, by introducing all necessary definitions. In next Sect. 3 we give a simple application of the interpolation method to the mean-field spin glass model. In particular, we show the sub-additivity of the quenched free energy with respect to the system size, and the existence of the infinite-volume limit [15].

Section 4 is devoted to a description of the main features of the Parisi representation for the free energy and to its rigorous establishment.

Section 5 will be devoted to some conclusion and outlook for future foreseen developments.

In conclusion, the author would like to thank the organizers of the 2006 Rio de Janeiro International Congress of Mathematical Physics, in particular Vladas Sidoravicius, for the kind invitation and exquisite hospitality to an event full of scientific, cultural and human content, in a so beautiful surrounding.

2 The Mean Field Spin Glass Model. Basic Definitions

As in the ferromagnetic mean field case, the generic configuration of the mean field spin glass model is defined through Ising spin variables $\sigma_i = \pm 1$, attached to each site $i = 1, 2, \ldots, N$.

But now there is also an external quenched disorder given by the $N(N-1)/2$ independent and identical distributed random variables J_{ij}, defined for each couple of sites. For the sake of simplicity, we assume each J_{ij} to be a centered unit Gaussian with averages $E(J_{ij}) = 0$, $E(J_{ij}^2) = 1$. By quenched disorder we mean that the J have a kind of stochastic external influence on the system, without participating to the thermal equilibrium.

Now the Hamiltonian of the model is given by the mean field expression

$$H_N(\sigma, J) = -\frac{1}{\sqrt{N}} \sum_{(i,j)} J_{ij}\sigma_i\sigma_j. \tag{1}$$

Here, the sum runs over all couples of sites. Notice that the term $\sqrt{N}$ is necessary in order to ensure a good thermodynamic behavior to the free energy, extensive in the system size. For the sake of simplicity, we have considered only the case of zero external field. But the general case, with a magnetic external field, can be treated without any essential additional complication.

For a given inverse temperature β, let us now introduce the disorder-dependent partition function $Z_N(\beta, J)$ and the quenched average of the free energy per site $f_N(\beta)$, according to the definitions

$$Z_N(\beta, J) = \sum_{\sigma_1 \ldots \sigma_N} \exp(-\beta H_N(\sigma, J)), \tag{2}$$

$$-\beta f_N(\beta) = N^{-1} E \log Z_N(\beta, J). \tag{3}$$

Notice that in (3) the average E with respect to the external noise is made *after* the log is taken. This procedure is called quenched averaging. It represents the physical idea that the external noise does not participate in the thermal equilibrium. Only the σ_i variables are thermalized.

For the sake of simplicity, it is also convenient to write the partition function in the following equivalent form. First of all let us introduce a family of centered Gaussian random variables $\mathscr{K}(\sigma)$, indexed by the configurations σ, and characterized by the covariances

$$E\big(\mathscr{K}(\sigma)\mathscr{K}(\sigma')\big) = q^2(\sigma, \sigma'), \tag{4}$$

where $q(\sigma, \sigma')$ are the overlaps between two generic configurations, defined by

$$q(\sigma, \sigma') = N^{-1} \sum_i \sigma_i\sigma_i', \tag{5}$$

with the obvious bounds $-1 \le q(\sigma, \sigma') \le 1$, and the normalization $q(\sigma, \sigma) = 1$. Then, starting from the definition (1), it is immediately seen that the partition function in (2) can be also written, by neglecting unessential constant terms, in the form

$$Z_N(\beta, \mathscr{K}) = \sum_{\sigma_1 \dots \sigma_N} \exp\left(\beta \sqrt{\frac{N}{2}} \mathscr{K}(\sigma)\right), \tag{6}$$

which will be the starting point of our treatment. Here the dependence of the partition function on the random variables $\mathscr{K}$ has been stressed in the notation.

According to the general well established strategy of statistical mechanics [26], firstly we consider the problem of the infinite volume limit.

3 The Thermodynamic Limit

In [15] we have given a very simple proof of a long awaited result, about the convergence of the free energy per site in the thermodynamic limit. Let us show the argument. Let us consider a system of size N and two smaller systems of sizes N_1 and N_2 respectively, with $N = N_1 + N_2$. Let us now compare

$$E \log Z_N(\beta, \mathscr{K}) = E \log \sum_{\sigma_1 \dots \sigma_N} \exp\left(\beta \sqrt{\frac{N}{2}} \mathscr{K}(\sigma)\right), \tag{7}$$

with

$$\begin{aligned} &E \log \sum_{\sigma_1 \dots \sigma_N} \exp\left(\beta \sqrt{\frac{N_1}{2}} \mathscr{K}_1(\sigma^{(1)})\right) \exp\left(\beta \sqrt{\frac{N_2}{2}} \mathscr{K}_2(\sigma^{(2)})\right) \\ &= E \log Z_{N_1}(\beta, \mathscr{K}_1) + E \log Z_{N_2}(\beta, \mathscr{K}_2), \end{aligned} \tag{8}$$

where $\sigma^{(1)}$ are the $(\sigma_i,\ i = 1, \dots, N_1)$, and $\sigma^{(2)}$ are the $(\sigma_i,\ i = N_1 + 1, \dots, N)$. Covariances for $\mathscr{K}_1$ and $\mathscr{K}_2$ are expressed as in (4), but now the overlaps are replaced with the partial overlaps of the first and second block, q_1 and q_2 respectively, defined as

$$q_1(\sigma, \sigma') = N_1^{-1} \sum_{i=1}^{N_1} \sigma_i \sigma_i', \tag{9}$$

and analogously for the q_2 of the second block.

The key idea now is to build an interpolation scheme, between the large system and the two small systems. This is easily achieved by introducing the interpolation parameter $0 \le t \le 1$, and the interpolating auxiliary function $\phi(t)$, defined as

$$\phi(t) = E \log \sum_{\sigma_1 \dots \sigma_N} \exp\left(\sqrt{t}\beta \sqrt{\frac{N}{2}} \mathscr{K} + \sqrt{1-t}\beta \sqrt{\frac{N_1}{2}} \mathscr{K}_1 + \sqrt{1-t}\beta \sqrt{\frac{N_2}{2}} \mathscr{K}_2\right). \tag{10}$$

Here, we have realized the families of random variables $\mathscr{K}$, $\mathscr{K}_1$, $\mathscr{K}_2$ as independent on the same probability space. The interpolation through the $\sqrt{t}$ and $\sqrt{1-t}$ assures a linear interpolation between the respective covariances. Obviously, we have

$$\phi(1) = E \log Z_N(\beta, \mathscr{K}),$$

while

$$\phi(0) = E \log Z_{N_1}(\beta, \mathscr{K}_1) + E \log Z_{N_2}(\beta, \mathscr{K}_2).$$

Now it is easy to calculate directly the t derivative of ϕ (see for example [13]), with the result

$$\frac{d}{dt}\phi(t) = \frac{\beta^2}{4}\frac{N_1 N_2}{N}\langle (q_1 - q_2)^2 \rangle_t, \tag{11}$$

where $\langle\rangle_t$ is a quite complicated, but explicitly given, t dependent probability measure on the random variables (q_1, q_2) [13]. In this derivation we have exploited the simple connection between the global overlap and the block overlaps

$$Nq = N_1 q_1 + N_2 q_2. \tag{12}$$

Since in any case the square in (11) is positive, by integrating on t and by exploiting the recognized boundary values at $t = 0$ and $t = 1$, we reach the super-additivity property

$$E \log Z_N(\beta, \mathscr{K}) \geq E \log Z_{N_1}(\beta, \mathscr{K}_1) + E \log Z_{N_2}(\beta, \mathscr{K}_2), \tag{13}$$

firstly established in [15]. Of course, the corresponding free energies show a sub-additive property, because of the minus sign involved in their definition.

From the superaddivity property, through standard methods [26], the existence of the limit follows in the form

$$\lim_{N\to\infty} N^{-1} E \log Z_N(\beta, \mathscr{K}) = \sup_N N^{-1} E \log Z_N(\beta, h, \mathscr{K}) \equiv -\beta f(\beta). \tag{14}$$

4 The Parisi Representation for the Free Energy

We refer to the original paper [25], and to the extensive review given in [20], for the general motivations, and the derivation of the broken replica *Ansatz*, in the frame of the ingenious replica trick. Here we limit ourselves to a synthetic description of its general structure, independently from the replica trick. The deep motivation for the introduction of the Parisi trial functional is sketched in [9], in the frame of the cavity method (see also [11]).

First of all, let us introduce the convex space $\mathscr{X}$ of the functional order parameters x, as nondecreasing functions of the auxiliary variable q, both x and q taking values on the interval [0, 1], i.e.

$$\mathscr{X} \ni x : [0, 1] \ni q \to x(q) \in [0, 1]. \tag{15}$$

Notice that we call x the function, and $x(q)$ its values. We introduce a metric on $\mathscr{X}$ through the $L^1([0, 1], dq)$ norm, where dq is the Lebesgue measure.

For our purposes, we will consider the case of piecewise constant functional order parameters, characterized by an integer K, and two sequences $q_0, q_1, \dots, q_K$, $m_1, m_2, \dots, m_K$ of numbers satisfying

$$0 = q_0 \le q_1 \le \cdots \le q_{K-1} \le q_K = 1, \qquad 0 \le m_1 \le m_2 \le \cdots \le m_K \le 1, \tag{16}$$

such that

$$x(q) = m_1 \quad \text{for } 0 = q_0 \le q < q_1, \qquad x(q) = m_2 \quad \text{for } q_1 \le q < q_2, \qquad \dots,$$
$$x(q) = m_K \quad \text{for } q_{K-1} \le q \le q_K. \tag{17}$$

In the following, we will find it convenient to define also $m_0 \equiv 0$, and $m_{K+1} \equiv 1$. The replica symmetric case of Sherrington and Kirkpatrick corresponds to

$$K = 2, \qquad q_1 = \bar{q}, \qquad m_1 = 0, \qquad m_2 = 1. \tag{18}$$

Let us now introduce the function f, with values $f(q, y; x, \beta)$, of the variables $q \in [0, 1]$, $y \in R$, depending also on the functional order parameter x, and on the inverse temperature β, defined as the solution of the nonlinear antiparabolic equation

$$(\partial_q f)(q, y) + \frac{1}{2}(\partial_y^2 f)(q, y) + \frac{1}{2}x(q)(\partial_y f)^2(q, y) = 0, \tag{19}$$

with final condition

$$f(1, y) = \log\cosh(\beta y). \tag{20}$$

Here, we have stressed only the dependence of f on q and y.

It is very simple to integrate (19) when x is piecewise constant. In fact, consider $x(q) = m_a$, for $q_{a-1} \le q \le q_a$, firstly with $m_a > 0$. Then, it is immediately seen that the correct solution of (19) in this interval, with the right final boundary condition at $q = q_a$, is given by

$$f(q, y) = \frac{1}{m_a} \log \int \exp\left(m_a f\left(q_a, y + z\sqrt{q_a - q}\,\right)\right) d\mu(z), \tag{21}$$

where $d\mu(z)$ is the centered unit Gaussian measure on the real line. On the other hand, if $m_a = 0$, then (19) loses the nonlinear part and the solution is given by

$$f(q, y) = \int f\left(q_a, y + z\sqrt{q_a - q}\,\right) d\mu(z), \tag{22}$$

which can be seen also to follow from (21) in the limit $m_a \to 0$. Starting from the last interval K, and using (21) iteratively on each interval, we easily get the solution of (19), (20), in the case of piecewise constant order parameter x, as in (17), through a chain of interconnected Gaussian integrations.

Now we introduce the following important definitions. The trial auxiliary function, associated to a given mean field spin glass system, as described in Sect. 3,

depending on the functional order parameter x, is defined as

$$\log 2 + f(0,0;x,\beta) - \frac{\beta^2}{2}\int_0^1 q\,x(q)\,dq. \tag{23}$$

Notice that in this expression the function f appears evaluated at $q = 0$, and $y = 0$.

The Parisi spontaneously broken replica symmetry expression for the free energy is given by the definition

$$-\beta f_P(\beta) \equiv \inf_x \left(\log 2 + f(0,0;x,\beta) - \frac{\beta^2}{2}\int_0^1 q\,x(q)\,dq \right), \tag{24}$$

where the infimum is taken with respect to all functional order parameters x.

Notice that the infimum appears here, as compared to the supremum that would appear in a variational principle of the usual entropy type in statistical mechanics. Therefore, Parisi variational principle is really a new structure in statistical mechanics, that deserves careful study in itself.

In [12], by exploiting a suitable interpolation, we have established a rigorous connection between the partition function of the mean field spin glass and the Parisi *Ansatz*.

The key point is to set up a useful interpolation scheme. This can be achieved as follows [12]. For a generic piece-wise constant order parameter as in (17), introduce a family of independent centered unit Gaussian random variables J_i^a, $a = 1,\dots,K$, $i = 1,\dots,N$. With the usual interpolation parameter $0 \le t \le 0$, introduce firstly the random variable

$$Z_K = \sum_{\sigma_1 \dots \sigma_N} \exp\left(\sqrt{t}\beta \sqrt{\frac{N}{2}}\mathscr{K}(\sigma) \right) \exp\left(\sqrt{1-t}\beta \sum_{a=1}^{K} \sqrt{q_a - q_{a-1}} \sum_i J_i^a \sigma_i \right). \tag{25}$$

Let us now denote by $E_K, E_{K-1}, \dots, E_0$ the averages with respect to $J_\cdot^K, J_\cdot^{K-1}, \dots, \mathscr{K}$, respectively. Then, starting from Z_K, define the random variables $Z_{K-1}, \dots, Z_1, Z_0$, recursively as follows

$$Z_{K-1}^{m_K} = E_K Z_K^{m_K} \tag{26}$$

$$Z_{a-1}^{m_a} = E_a Z_a^{m_a} \tag{27}$$

$$Z_0^{m_1} = E_1 Z_1^{m_1}, \tag{28}$$

and the interpolating function $\phi(t) = N^{-1} E_0 \log Z_0$.

It is simple to verify that at the boundary values for t we have

$$\phi(1) = N^{-1} E \log Z(\beta, \mathscr{K})$$

for $t = 1$, where the partition function defined in (6) appears, while for $t = 0$, the repeated integrations over the J variables give precisely

$$\phi(0) = \log 2 + f(0, 0; x, \beta),$$

which is one piece of the Parisi representation.

At this point, we can calculate the t derivative through a series of long but straightforward steps. Some miracles show up. Upon integration on t, we reach the final result in the form of a sum rule

$$\log 2 + f(0, 0; x, \beta) - \frac{\beta^2}{2} \int_0^1 q\, x(q)\, dq$$
$$= N^{-1} E \log Z_N(\beta, \mathscr{K}) + \frac{\beta^2}{4} \langle (q_{12} - q_a)^2 \rangle, \tag{29}$$

where $\langle\rangle$ is an explicitly given but quite complicated measure average over the variables σ, σ', appearing in the two replica overlap q_{12}, and the variable $q_.$, taking the values q_a. The sum rule holds for any value of the order parameter x. One of the miracles occurring in the proof of this sum rule is that the second term appearing in the Parisi trial functional here comes for free from the completion of the square in the third term of the sum rule.

In any case, the third term, being the average of a square, is positive. Therefore we have the following important result.

Theorem 1. *For all values of the inverse temperature β, and for any functional order parameter x, the following bound holds*

$$N^{-1} E \log Z_N(\beta, \mathscr{K}) \leq \log 2 + f(0, 0; x, \beta) - \frac{\beta^2}{2} \int_0^1 q\, x(q)\, dq,$$

uniformly in N. Consequently, we have also

$$N^{-1} E \log Z_N(\beta, \mathscr{K}) \leq \inf_x \left(\log 2 + f(0, h; x, \beta) - \frac{\beta^2}{2} \int_0^1 q\, x(q)\, dq \right),$$

uniformly in N.

This result can be understood also in the frame of the generalized variational principle established by Aizenman-Sims-Starr [1], as shown for example in [13], by exploiting the general structure of the Derrida-Ruelle-Parisi probability cascades.

Up to this point we have seen how to obtain upper bounds. The problem arises whether, as for example can be easily seen in the ferromagnetic case [13], we can also get lower bounds, so as to shrink the thermodynamic limit to the value given by the $\inf_x$ in Theorem 1. After a short announcement in [30], Michel Talagrand wrote an extended paper [32], where the complete proof of the control of the lower bound is firmly established. We refer to the original paper for the complete details of this remarkable achievement. About the methods, here we only recall that the sum rule in [12], explained above, gives also the corrections to the bounds appearing in Theorem 1, albeit in a quite complicated form. Talagrand has been able to establish that these corrections do in fact vanish in the thermodynamic limit. In order to be

able to reach this important result it is necessary to prove an extension of the broken replica symmetry bounds of Theorem 1 to the case where two replicas of the system are coupled together. This task has not been reached yet in its full generality, but the treatment given by Talagrand is sufficient to prove the vanishing of the correction terms in the infinite volume limit.

In conclusion, we can establish the following conclusive result about the expression of the free energy in the mean field spin glass.

Theorem 2. *For the mean field spin glass model we have*

$$\lim_{N\to\infty} N^{-1} E \log Z_N(\beta, \mathscr{K}) = \sup_N N^{-1} E \log Z_N(\beta, \mathscr{K}) \tag{30}$$

$$= \inf_x \left(\log 2 + f(0, 0; x, \beta) - \frac{\beta^2}{2} \int_0^1 q\, x(q)\, dq \right). \tag{31}$$

This is the main result obtained up to now in the mathematical treatment of the mean field spin glass model.

5 Conclusion and Outlook for Future Developments

As we have seen, in these last few years there has been an impressive progress in the understanding of the mathematical structure of spin glass models, mainly due to the systematic exploitation of interpolation methods. However many important problems are still open. The most important one is to establish rigorously the full hierarchical ultrametric organization of the overlap distributions, as appears in Parisi theory, and to fully understand the decomposition in pure states of the glassy phase, at low temperatures. Some partial steps in this direction have been obtained through the establishment of the so called Ghirlanda-Guerra identities [14], but the general solution seems to be quite far.

Moreover, is would be useful to extend these methods to other important disordered models, such as for example neural networks. Here the difficulty is that the positivity arguments, so essential in the application of the interpolation methods, do not seem to emerge naturally inside the structure of the theory. Even for a class of simple mean field diluted ferromagnetic systems, the treatment of the infinite volume limit has not been reached yet, due to the lack of positivity arguments. Only the $\beta \to \infty$ limit is well understood [4].

For extensions to diluted spin glass models we refer for example to [6, 17, 24, 3].

Finally, the problem of connecting properties of the short-range model with those arising in the mean field case is still almost completely open. For partial results, and different points of view, see [16, 7, 8, 19, 21, 23].

Recently a pedagogically very useful complete review appeared [2], about the application of the interpolation methods, and the other methods of spin glass theory, to the simple case of the ferromagnetic mean field model.

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Surface Operators and Knot Homologies

Sergei Gukov

Abstract Topological gauge theories in four dimensions which admit surface operators provide a natural framework for realizing homological knot invariants. Every such theory leads to an action of the braid group on branes on the corresponding moduli space. This action plays a key role in the construction of homological knot invariants. We illustrate the general construction with examples based on surface operators in $\mathcal{N} = 2$ and $\mathcal{N} = 4$ twisted gauge theories which lead to a categorification of the Alexander polynomial, the equivariant knot signature, and certain analogs of the Casson invariant.

1 Introduction

Topological field theory is a natural framework for "categorification", an informal procedure that turns integers into vector spaces (Abelian groups), vector spaces into Abelian or triangulated categories, operators into functors between these categories [14]. The number becomes the dimension of the vector space, while the vector space becomes the Grothendieck group of the category (tensored with a field). This procedure can be illustrated by the following diagram [29]: Recently, this idea led to

$$\text{Number} \underset{\text{dimension}}{\overset{\text{Categorification}}{\rightleftarrows}} \text{Vector Space} \underset{\text{Grothendieck Group}}{\overset{\text{Categorification}}{\rightleftarrows}} \text{Category}$$

a number of remarkable developments in various branches of mathematics, notably in low-dimensional topology, where many polynomial knot invariants were lifted to homological invariants.

Sergei Gukov
Department of Physics, University of California, Santa Barbara, CA 93106, USA,
e-mail: gukov@theory.caltech.edu

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Although the list of homological knot invariants is constantly growing, most of the existing knot homologies fit into the "A-series" of homological knot invariants associated with the fundamental representation of $sl(N)$ (or $gl(N)$). Each such theory is a doubly graded knot homology whose graded Euler characteristic with respect to one of the gradings gives the corresponding knot invariant,

$$P(q) = \sum_{i,j} (-1)^i q^j \dim \mathscr{H}_{i,j}. \tag{1}$$

For example, the Jones polynomial can be obtained in this way as the graded Euler characteristic of the Khovanov homology [37]. Similarly, the so-called knot Floer homology [62, 64] provides a categorification of the Alexander polynomial $\Delta(q)$. At first, these as well as other homological knot invariants listed in the table below appear to have very different character. Thus, as the name suggests, knot Floer homology is defined as a symplectic Floer homology of two Lagrangian submanifolds in a certain configuration space, while the other theories are defined combinatorially. In addition, the definition of the knot Floer homology admits a generalization to knots in arbitrary 3-manifolds, whereas at present the definition of the other knot homologies (with $N > 0$) is known only for knots in $\mathbf{R}^3$.

Table 1 A general picture of knot polynomials and knot homologies

$\mathfrak{g}$	Knot Polynomial	Categorification
$gl(1\|1)$	$\Delta(q)$	knot Floer homology $HFK(K)$
"$sl(1)$"	–	Lee's deformed theory $H'(K)$
$sl(2)$	Jones	Khovanov homology $H^{\mathrm{Kh}}(K)$
$sl(N)$	$P_N(q)$	$sl(N)$ homology $HKR^N(K)$

The $sl(N)$ knot homology [37, 39, 41]—whose Euler characteristic is the quantum $sl(N)$ invariant $P_N(q)$—has a physical interpretation as the space of BPS states, $\mathscr{H}_{BPS}$, in string theory [22]. In order to remind the physical setup of [22], let us recall that polynomial knot invariants, such as $P_N(q)$, can be related to open topological string amplitudes ("open Gromov-Witten invariants") by first embedding Chern-Simons gauge theory in topological string theory [75], and then using the so-called large N duality [17, 18, 60, 49], a close cousin of the celebrated AdS/CFT duality [54]. Moreover, open topological string amplitudes and, hence, the corresponding knot invariants can be reformulated in terms of new integer invariants which capture the spectrum of BPS states in the string Hilbert space, $\mathscr{H}_{BPS}$. The BPS states in question are membranes ending on Lagrangian five-branes in M-theory on a non-compact Calabi-Yau space $\mathbf{X} = \mathscr{O}_{\mathbf{P}^1}(-1) \oplus \mathscr{O}_{\mathbf{P}^1}(-1)$. Specifically, the five-branes have world-volume $\mathbf{R}^{2,1} \times L_K$ where $L_K \subset \mathbf{X}$ is a Lagrangian submanifold (which depends on knot K) and $\mathbf{R}^{2,1} \subset \mathbf{R}^{4,1}$.

Surprisingly, the physical interpretation of the $sl(N)$ knot homology naturally leads to a triply-graded (rather than doubly-graded) knot homology [22] (see also

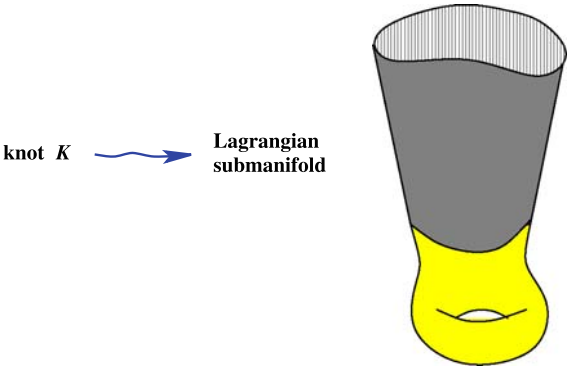


Fig. 1 A membrane ending on a Lagrangian five-brane

[20, 23]). Indeed, the Hilbert space of BPS states, $\mathscr{H}_{BPS}$, is graded by three quantum numbers, which are easy to see in the physical setup described in the previous paragraph. The world-volume of the five-brane breaks the $SO(4) \cong SU(2) \times SU(2)$ rotation symmetry in five dimensions down to a subgroup $U(1)_L \times U(1)_R$, where $U(1)_L$ (resp. $U(1)_R$) is a rotation symmetry in the dimensions parallel (resp. transverse) to the five-brane. Therefore, BPS states in the effective $\mathscr{N} = 2$ theory on the five-brane are labeled by three quantum numbers j_L, j_R, and Q, where $Q \in H_2(\mathbf{X}, L_K) \cong \mathbb{Z}$ is the relative homology class represented by the membrane world-volume. In other words, apart from the $\mathbb{Z}_2$-grading by the fermion number, the Hilbert space of BPS states $\mathscr{H}_{BPS}$ is triply-graded. The properties of this triply-graded theory were studied in [15]; it turns out that this theory unifies all the doubly-graded knot homologies listed in Table 1, including the knot Floer homology. A mathematical definition of the triply-graded knot homology which appears to have many of the expected properties was constructed in [42].

Apart from realization in (topological) string theory, the homological knot invariants are expected to have a physical realization also in topological gauge theory, roughly as polynomial knot invariants have a physical realization in three-dimensional gauge theory (namely, in the Chern-Simons theory [73]) as well as in the topological string theory [75, 17, 18, 60]. Although these two realizations are not unrelated, different properties of knot polynomials are easier to see in one description or the other. For example, the dependence on the rank N is manifest in the string theory description, while the skein operations and transformations under surgeries are easier to see in the Chern-Simons gauge theory.

Similarly, as we explained above, string theory realization is very useful for understanding relation between knot homologies of different rank. On the other hand, the formal properties of knot homologies which are hard to see in string theory (which, however, would be very natural in topological field theory) have to do with the fact that, in most cases, knot homologies can be extended to a functor $\mathscr{F}$ from the category of 3-manifolds with links and cobordisms to the category of graded vector spaces and homomorphisms

$$\mathscr{F}(Y;\, K) = \mathscr{H}_{Y;K} \tag{2}$$

$$\mathscr{F}(X;\, D) \;:\; \mathscr{H}_{Y;K} \to \mathscr{H}_{Y';K'} \tag{3}$$

Moreover, on manifolds with corners, it is expected that $\mathscr{F}$ extends to a 2-functor from the 2-category of oriented and decorated 4-manifolds with corners to the 2-category of triangulated categories [38, 34, 2]. In particular, it should associate:

- A triangulated category $\mathscr{F}(\Sigma)$ to a closed oriented 2-manifold Σ;
- An exact functor $\mathscr{F}(Y)$ to a 3-dimensional oriented cobordism Y;
- A natural transformation $\mathscr{F}(X)$ to a 4-dimensional oriented cobordism X.

As we explain below, these are precisely the formal properties of a four—dimensional topological field theory with boundaries and corners. Moreover, links and link cobordisms can be incorporated by introducing "surface operators" in the topological gauge theory.

In Sect. 2, we discuss the general aspects of topological gauge theories which admit surface operators. Of particular importance is the fact that every topological gauge theory which admits surface operators gives rise to an action of the braid group on D-branes. Then, in Sects. 3 and 4 we illustrate how these general structures are realized in simple examples of $\mathcal{N} = 2$ and $\mathcal{N} = 4$ twisted gauge theories. Specifically, in Sect. 3 we study surface operators and the corresponding knot homologies in the Donaldson-Witten theory and in the Seiberg-Witten theory, both of which are obtained by twisting $\mathcal{N} = 2$ supersymmetric gauge theory. In Sect. 4, we explain that a particular twist of the $\mathcal{N} = 4$ super-Yang-Mills theory—studied recently in connection with the geometric Langlands program [36, 21]—with a simple type of surface operators provides a physical framework for categorification of the $G_{\mathbf{C}}$ Casson invariant.

2 Gauge Theory and Categorification

Let us start by describing the general properties of the topological quantum field theory (TQFT) with boundaries, corners, and surface operators. To a closed 4-manifold X, a four-dimensional TQFT associates a number, $Z(X)$, the partition function of the topological theory on X. Similarly, to a closed 3-manifold Y, it associates a vector space, $\mathscr{H}_Y$, the Hilbert space obtained by quantization of the theory on $X = \mathbf{R} \times Y$. Finally, to a closed surface Σ it associates a triangulated category, $\mathscr{F}(\Sigma)$, which can be understood as the category of D-branes in the topological sigma-model obtained via the dimensional reduction of gauge theory on Σ. The objects of the category $\mathscr{F}(\Sigma)$ describe BRST-invariant boundary conditions in the four-dimensional TQFT on 4-manifolds with corners (locally, such manifolds look like $X = \mathbf{R} \times \mathbf{R}_+ \times \Sigma$). Summarizing,

gauge theory on X	$\rightsquigarrow$	number $Z(X)$
gauge theory on $\mathbf{R} \times Y$	$\rightsquigarrow$	vector space $\mathscr{H}_Y$
gauge theory on $\mathbf{R}^2 \times \Sigma$	$\rightsquigarrow$	category $\mathscr{F}(\Sigma)$

where we assume that X, Y, and Σ are closed. Depending on whether the topological reduction of the four-dimensional gauge theory on $\mathbf{R}^2 \times \Sigma$ gives a topological A-model or B-model, the category $\mathscr{F}(\Sigma)$ is either the derived Fukaya category,[1] $\mathbf{Fuk}(\mathscr{M})$, or the derived category of coherent sheaves, $D^b(\mathscr{M}) := D^b\mathbf{Coh}(\mathscr{M})$,

$$\begin{array}{ll} \text{topological A-model:} & \mathscr{F}(\Sigma) = \mathbf{Fuk}(\mathscr{M}) \\ \text{topological B-model:} & \mathscr{F}(\Sigma) \;=\; D^b(\mathscr{M}) \end{array}$$

where $\mathscr{M}$ is the moduli space of classical solutions in gauge theory on $\mathbf{R}^2 \times \Sigma$, invariant under translations along $\mathbf{R}^2$. Different topological gauge theories lead to different functors $\mathscr{F}$. For example, in the context of Donaldson-Witten theory [72], Fukaya suggested [16] that the category associated to a closed surface Σ should be A_∞-category of Lagrangian submanifolds in the moduli space of flat G-connections on Σ. This is precisely what one finds from the topological reduction [3] of the twisted $\mathscr{N} = 2$ gauge theory on $\mathbf{R}^2 \times \Sigma$, in agreement with the general principle discussed here.

The Atiyah-Floer Conjecture and Its Variants

It is easy to see that $\mathscr{F}$ defined by the topological gauge theory has all the expected properties of a 2-functor. In particular, to a 3-manifold Y with boundary $\partial Y = \Sigma$ it associates a "D-brane", that is an object in the category $\mathscr{F}(\Sigma)$.

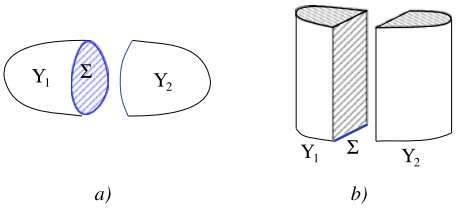


Fig. 2 (a) A 3-manifold Y can be obtained as a connected sum of 3-manifolds Y_1 and Y_2, joined along their common boundary Σ. (b) In four-dimensional gauge theory, the space $\mathbf{R} \times Y$ is obtained by gluing two 4-manifolds with corners

The interpretation of 3-manifolds with boundary as D-branes can be used to reproduce the Atiyah-Floer conjecture, which states [1]:

$$HF_*^{\text{inst}}(Y) \cong HF_*^{\text{symp}}(\mathscr{M}; \mathscr{L}_1, \mathscr{L}_2) \tag{4}$$

Here $\mathscr{M} = \mathscr{M}_{flat}^G$ is the moduli space of flat connections on Σ, while $\mathscr{L}_1$ and $\mathscr{L}_2$ are Lagrangian submanifolds in $\mathscr{M}$ associated with the Heegard splitting of Y,

$$Y = Y_1 \cup_\Sigma Y_2 \tag{5}$$

[1] Notice, according to the Homological Mirror Symmetry conjecture, this category is equivalent to the derived category of the mirror B-model [44]. In particular, the category $\mathbf{Fuk}(\mathscr{M})$, suitably defined, must be a triangulated category [7].

such that the points of $\mathscr{L}_i \subset \mathscr{M}$, $i = 1, 2$, correspond to flat connections on Σ which can be extended to Y_i.

Similarly, in the B-model, Y_1 and Y_2 define the corresponding B-branes, which are objects in the derived category of coherent sheaves on $\mathscr{M}$. In both cases, the vector space $\mathscr{H}_Y$ associated with the compact 3-manifold Y is the space of "1–2 strings":

$$\mathscr{H}_Y = \begin{cases} HF_*^{\text{symp}}(\mathscr{M}; \mathscr{L}_1, \mathscr{L}_2) & \text{A-model} \\ \text{Ext}^*(\mathscr{F}_{Y_1}, \mathscr{F}_{Y_2}) & \text{B-model} \end{cases} \tag{6}$$

In the Donaldson-Witten theory, this leads to the Atiyah-Floer conjecture (4).

"*Decategorification*"

The operation represented by the arrow going to the left in (1)—"decategorification"—also has a natural interpretation in gauge theory. It corresponds to the dimensional reduction, or compactification on a circle. Indeed, the partition function in gauge theory on $X = \mathbf{S}^1 \times Y$ is the trace (the index) over the Hilbert space $\mathscr{H}_Y$:

$$Z_{\mathbf{S}^1 \times Y} = \chi(\mathscr{H}_Y) \tag{7}$$

Similarly, the vector space associated with $Y = \mathbf{S}^1 \times \Sigma$ is the Grothendieck group of the category $\mathscr{F}(\Sigma)$

$$\mathscr{H}_{\mathbf{S}^1 \times \Sigma} = K(\mathscr{F}(\Sigma)) \tag{8}$$

In the case of A-model and B-model, respectively, we find

$$K(\mathscr{F}(\Sigma)) = \begin{cases} H^d(\mathscr{M}) & \text{for } \mathscr{F}(\Sigma) = \mathbf{Fuk}(\mathscr{M}) \\ H^*(\mathscr{M}) & \text{for } \mathscr{F}(\Sigma) = D^b(\mathscr{M}) \end{cases} \tag{9}$$

where $d = \frac{1}{2}\dim(\mathscr{M})$.

2.1 Incorporating Surface Operators

In a three-dimensional TQFT, knots and links can be incorporated by introducing topological loop observables. The familiar example is the Wilson loop observable in Chern-Simons theory,

$$W_R(K) = \text{Tr}_R\left(P \exp \oint_K A\right) \tag{10}$$

Recall, that canonical quantization of the Chern-Simons theory on $\Sigma \times \mathbf{R}$ associates a vector space $\mathscr{H}_\Sigma$—the "physical Hilbert space"—to a Riemann surface Σ [73]. In presence of Wilson lines, quantization gives a Hilbert space $\mathscr{H}_{\Sigma; p_i, R_i}$ canonically associated to a Riemann surface Σ together with marked points p_i (points where Wilson lines meet Σ) decorated by representations R_i. For example, to n

marked points on the plane colored by the fundamental representation it associates $\mathfrak{V}^{\otimes n}$, where $\mathfrak{V}$ is a N-dimensional irreducible representation of the quantum group $U_q(sl(N))$.

We wish to lift this to a four-dimensional gauge theory by including the "time" direction, so that the space-time becomes $X = Y \times \mathbf{R}$, where the knot K is represented by a topological defect (which was called a "surface operator" in [21]) localized on the surface $D = K \times \mathbf{R}$. In the Feynman path integral, a surface operator is defined by requiring the gauge field A (and perhaps other fields as well) to have a prescribed singularity. For example, the simplest type of singularity studied in [21] creates a holonomy of the gauge field on a small loop around D,

$$V = \mathrm{Hol}(A) \tag{11}$$

Quantization of the four-dimensional topological theory on a 4-manifold $X = Y \times \mathbf{R}$ with a surface operator on $D = K \times \mathbf{R}$ gives rise to a functor that associates to this data (namely, a 3-manifold Y, a knot K, and parameters of the surface operator) a vector space, the space of quantum ground states,

$$\mathscr{F}(Y; K) = \mathscr{H}_{Y;K,\text{parameters}} \tag{12}$$

Moreover, we will be interested in surface operators which preserve topological invariance for more general 4-manifolds X and embedded surfaces $D \subset X$. For example, if the four-dimensional topological gauge theory is obtained by a topological twist of a supersymmetric gauge theory, it is natural to consider a special class of surface operators which preserve supersymmetry, in particular, those supercharges which become BRST charges in the twisted theory. Such surface operators can be defined on a more general embedded surface D, which might be either closed or end on the boundary of X. An example of this situation is a four-dimensional TQFT with corners, shown on Fig. 3, which arises when we consider a lift of a 3-manifold with boundary Σ and line operators with end-points on Σ.

To summarize, including topological surface operators in the four-dimensional gauge theory, we obtain a functor from the category of 3-manifolds with links and their cobordisms to the category of graded vector spaces and homomorphisms:

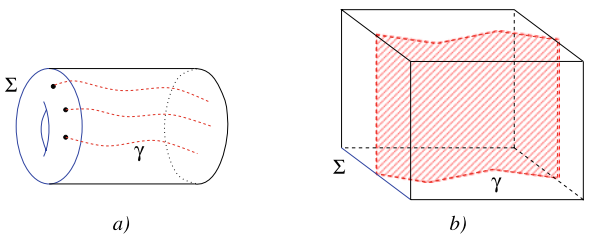


Fig. 3 (a) Line operators in a three-dimensional TQFT on $\Sigma \times I$ and (b) topological "surface operators" in four-dimensional gauge theory on $\Sigma \times I \times \mathbf{R}$

$$\mathscr{F}(X;\, D)\ :\ \mathscr{H}_{Y;K} \to \mathscr{H}_{Y';K'} \tag{13}$$

Here, the knot homology $\mathscr{H}_{Y;K}$ is the space of quantum ground states in the four-dimensional gauge theory with surface operators and boundaries. Similarly, the functor $\mathscr{F}$ associates a number (the partition function) to a closed 4-manifold with embedded surfaces, and a category $\mathscr{F}(\Sigma;\, p_i)$ to a surface Σ with marked points, p_i, which correspond to the end-points of the topological surface operators.

As in the theory without surface operators, the category $\mathscr{F}(\Sigma;\, p_i)$ is either the category of A-branes or the category of B-branes on $\mathscr{M}$, depending on whether the topological reduction of the four-dimensional gauge theory is A-model or B-model. Here, $\mathscr{M}$ is the moduli space of $\mathbf{R}^2$-invariant solutions in gauge theory on $X = \mathbf{R}^2 \times \Sigma$ with surface operators supported at $\mathbf{R}^2 \times p_i$.

2.2 Braid Group Actions

As we just explained, surface operators are the key ingredients for realizing knot homologies in four-dimensional gauge theory. Our next goal is to explain that every topological gauge theory which admits surface operators is, in a sense, a factory that produces examples of braid group actions on branes, including some of the known examples as well as the new ones.[2]

In general, the mapping class group of the surface Σ acts on branes on $\mathscr{M}$. In particular, when Σ is a plane with n punctures, the moduli space $\mathscr{M}$ is fibered over the configuration space $\mathrm{Conf}^n(\mathbb{C})$ of n unordered points on $\mathbb{C}$,

$$\begin{array}{c} \mathscr{M} \\ \downarrow \\ \mathrm{Conf}^n(\mathbb{C}) \end{array} \tag{14}$$

and the braid group $Br_n = \pi_1(\mathrm{Conf}^n(\mathbb{C}))$ (= the mapping class group of the n-punctured disk) acts on the category $\mathscr{F}(\Sigma)$. Recall, that the braid group on n strands, Br_n, has $n-1$ generators, σ_i, $i = 1, \ldots, n-1$ which satisfy the following relations

$$\sigma_i \sigma_{i+1} \sigma_i = \sigma_{i+1} \sigma_i \sigma_{i+1} \tag{15}$$

$$\sigma_i \sigma_j = \sigma_j \sigma_i, \quad |i-j| > 1 \tag{16}$$

where σ_i can be represented by a braid with only one crossing between the strands i and $i+1$, as shown on the figure below.

In gauge theory, the action of the braid group on branes is induced by braiding of the surface operators. Namely, a braid, such as the one on Fig. 4, corresponds

[2] It is worth pointing out that, compared to [21], where the braid group action is associated with *local* singularities in the moduli space $\mathscr{M}$, in the present context the origin of the braid group action is associated with *global* singularities.

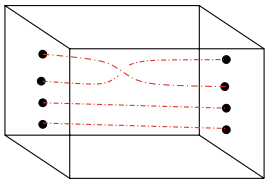


Fig. 4 A braid on four strands

to a non-contractible loop in the configuration space, $\mathrm{Conf}^n(\mathbb{C})$. As we go around the loop, the fibration (14) has a monodromy, which acts on the category of branes $\mathscr{F}(\Sigma)$ as an autoequivalence,

$$Br_n \to \mathrm{Auteq}(\mathscr{F}(\Sigma)) \tag{17}$$

$$\beta \mapsto \phi_\beta \tag{18}$$

The simplest situation where one finds the action of the braid group Br_n on A-branes (resp. B-branes) on $\mathscr{M}$ is when $\mathscr{M}$ contains A_{n-1} chain of Lagrangian spheres (resp. spherical objects).

We remind that an A_{n-1} chain of Lagrangian spheres is a collection of Lagrangian spheres $\mathscr{L}_1, \ldots, \mathscr{L}_{n-1} \subset \mathscr{M}$, such that

$$\#(\mathscr{L}_i \cap \mathscr{L}_j) = \begin{cases} 1 & |i-j| = 1 \\ 0 & |i-j| > 1 \end{cases} \tag{19}$$

These configurations occur when $\mathscr{M}$ can be degenerated into a manifold with singularity of type A_{n-1}. Indeed, to any Lagrangian sphere $\mathscr{L} \subset \mathscr{M}$, one can associate a symplectic automorphism of $\mathscr{M}$, the so-called generalized Dehn twist $T_{\mathscr{L}}$ along $\mathscr{L}$, which acts on $H_*(\mathscr{M})$ as the Picard-Lefschetz monodromy transformation

$$(T_{\mathscr{L}})_*(x) = \begin{cases} x - ([\mathscr{L}] \cdot x)[\mathscr{L}] & \text{if } \dim(x) = \dim(\mathscr{L}) \\ x & \text{otherwise} \end{cases} \tag{20}$$

As shown in [68], Dehn twists $T_{\mathscr{L}_i}$ along A_{n-1} chains of Lagrangian spheres satisfy the braid relations (15), and this induces an action of the braid group with n strands on the category of A-branes, $\mathbf{Fuk}(\mathscr{M})$.

The mirror of this construction gives an example of the braid group action on B-branes [70]. In this case, the braid group is generated by the twist functors along spherical objects ("spherical B-branes") which are mirror to the Lagrangian spheres. As the name suggests, an object $\mathscr{E} \in D^b(\mathscr{M})$ is called d-spherical if $\mathrm{Ext}^*(\mathscr{E}, \mathscr{E})$ is isomorphic to $H^*(S^d, \mathbb{C})$ for some $d > 0$,

$$\mathrm{Ext}^i(\mathscr{E}, \mathscr{E}) = \begin{cases} \mathbb{C} & \text{if } i = 0 \text{ or } d \\ 0 & \text{otherwise} \end{cases} \tag{21}$$

A spherical B-brane defines a twist functor $T_{\mathscr{E}} \in \mathrm{Auteq}(D^b(\mathscr{M}))$ which, for any $\mathscr{F} \in D^b(\mathscr{M})$, fits into exact triangle

$$\mathrm{Hom}^*(\mathscr{E}, \mathscr{F}) \otimes \mathscr{E} \longrightarrow \mathscr{F} \longrightarrow T_{\mathscr{E}}(\mathscr{F}) \tag{22}$$

where the first map is evaluation. At the level of D-brane charges, the twist functor $T_{\mathscr{E}}$ acts as, cf. (20),

$$x \mapsto x + (v(\mathscr{E}) \cdot x)\, v(\mathscr{E})$$

where $v(\mathscr{E}) = ch(\mathscr{E})\sqrt{Td(\mathscr{M})} \in H^*(\mathscr{M})$ is the D-brane charge (the Mukai vector) of $\mathscr{E}$.

The mirror of an A_{n-1} chain of Lagrangian spheres is an A_{n-1} chain of spherical objects, that is a collection of spherical objects $\mathscr{E}_1, \ldots, \mathscr{E}_{n-1}$ which satisfy the condition analogous to (19),

$$\sum_k \dim \mathrm{Ext}^k(\mathscr{E}_i, \mathscr{E}_j) = \begin{cases} 1 & |i-j| = 1 \\ 0 & |i-j| > 1 \end{cases} \tag{23}$$

With some minor technical assumptions [70], the corresponding twist functors $T_{\mathscr{E}_i}$ generate an action of the braid group Br_n on $D^b(\mathscr{M})$. As we illustrate below, many examples of braid group actions on branes can be found by studying gauge theory with surface operators.

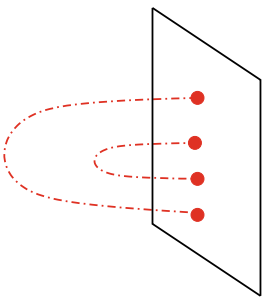


Fig. 5 A particular brane $\widetilde{\mathscr{B}}$ which corresponds to closing a braid on four strands

In A-model as well as in B-model, the braid group action on branes can be used to write a convenient expression for knot homology, $\mathscr{H}_K$, of a knot K represented as a braid closure. Let K be a knot obtained by closing a braid β on both ends as shown on Fig. 5. Then, the space of quantum ground states, $\mathscr{H}_K$, in the four-dimensional gauge theory with a surface operator on $D = \mathbf{R} \times K$ can be represented as the space of open string states between branes $\widetilde{\mathscr{B}}$ and $\widetilde{\mathscr{B}}' = \phi_\beta(\widetilde{\mathscr{B}})$. Here, $\widetilde{\mathscr{B}}$ is the basic brane which corresponds to the configuration on Fig. 5, while $\widetilde{\mathscr{B}}'$ is the brane obtained from it by applying the functor ϕ_β; it corresponds to the braid β closed on one side. These are A-branes (resp. B-branes) in the case of A-model (resp. B-

model), and the space open strings is, *cf.* (6),

$$\mathscr{H}_K = \begin{cases} HF_*^{\text{symp}}(\mathscr{M}; \widetilde{\mathscr{B}}, \phi_\beta(\widetilde{\mathscr{B}})) & \text{A-model} \\ \text{Ext}^*(\widetilde{\mathscr{B}}, \phi_\beta(\widetilde{\mathscr{B}})) & \text{B-model} \end{cases} \tag{24}$$

In particular, when topological reduction of the gauge theory gives A-model, the branes $\widetilde{\mathscr{B}}$ and $\widetilde{\mathscr{B}}'$ are represented by Lagrangian submanifolds in $\mathscr{M}$. This leads to a construction of link homologies via symplectic geometry, as in [69, 55, 56].

3 Surface Operators and Knot Homologies in $\mathscr{N} = 2$ Gauge Theory

Now, let us illustrate the general structures discussed in the previous section in the context of $\mathscr{N} = 2$ topological gauge theory in four dimensions. For simplicity, we consider examples of $\mathscr{N} = 2$ gauge theories with gauge groups $G = SU(2)$ and $G = U(1)$ known as the Donaldson-Witten theory and the Seiberg-Witten theory, respectively. In fact, these two theories are closely related [67]—the former describes the low-energy physics of the latter—and below we shall use this fact to compare the corresponding knot homologies.

3.1 Donaldson-Witten Theory and the Equivariant Knot Signature

We start with pure $\mathscr{N} = 2$ super-Yang-Mills theory with gauge group G which for simplicity we take to be $SU(2)$. After the topological twist, the $\mathscr{N} = 2$ gauge theory can be formulated on arbitrary 4-manifold X and localizes on the anti-self-dual ("instanton") field configurations [72]:

$$F_A^+ = 0 \tag{25}$$

The space of quantum ground states on $\mathbf{R} \times Y$ is the instanton Floer homology defined[3] by studying the gradient flow of the Chern-Simons functional,

$$\mathscr{H}_Y = HF_*^{\text{inst}}(Y) \tag{26}$$

and the topological reduction [3] on $\mathbf{R}^2 \times \Sigma$ leads to a topological A-model with the target space $\mathscr{M} = \mathscr{M}_{flat}^G$, the moduli space of flat connections on Σ. As we already mentioned in the previous section these facts, together with the interpretation of boundaries as D-branes, naturally lead to the statement of the Atiyah-Floer conjecture. The Euler characteristic of $\mathscr{H}_Y$ is the Casson invariant, $\lambda_G(Y)$, which

[3] As in the original Floer's definition, we mainly assume that Y is a homology sphere when we talk about $HF_*^{\text{inst}}(Y)$ in order to avoid difficulties related to reducible connections.

computes the Euler characteristic of the moduli space of flat G-connections on Y,

$$\chi(\mathscr{H}_Y) = 4\lambda_G(Y) \tag{27}$$

In the special case of $G = SU(2)$ that we are mainly considering here, it is the standard Casson-Walker-Lescop invariant $\lambda_{CWL}(Y)$ which sometimes we write simply as $\lambda(Y)$.

We note that, while the homological invariant $\mathscr{H}_Y$ is difficult to study on 3-manifolds with $b_1 > 1$, its Euler characteristic—which is, at least formally, computed by the partition function of the four-dimensional gauge theory on $X = \mathbf{S}^1 \times Y$—is still given by the Casson invariant [57],

$$Z_{DW}(\mathbf{S}^1 \times Y) = 4\lambda \tag{28}$$

Since $b_2^+(X) = b_1(Y)$ for $X = \mathbf{S}^1 \times Y$, computing (28) is much easier in the case $b_1(Y) > 1$. Indeed, in general the Donaldson-Witten partition function $Z_{DW}(X)$ can be written as a sum of the contribution of the Coulomb branch (the u-plane integral) and two contributions, Z_M and Z_D, both of which are described by the Seiberg-Witten theory (that we consider in more detail below):

$$Z_{DW} = Z_u + Z_M + Z_D \tag{29}$$

For manifolds $X = \mathbf{S}^1 \times Y$ with $b_1(Y) > 1$ the u-plane integral vanishes and we have $Z_M = Z_D = 2\lambda(Y)$, which then add up to (27). If $b_1(Y) = 1$, the Donaldson-Witten partition function $Z_{DW}(\mathbf{S}^1 \times Y)$ depends on the metric. In particular, it should be compared with the Euler characteristic of $\mathscr{H}_Y$ in the chamber $R \to \infty$, where R is the radius of $\mathbf{S}^1$. In this case, the u-plane integral is non-zero, and instead of (28) one finds a similar expression with the "correction" $-\frac{4}{6}|\mathrm{Tor}H_1(Y, \mathbb{Z})|$, see [57] for more details.

Surface Operators

Now let us consider surface operators in the Donaldson-Witten theory which correspond to the singularity of the gauge field of the form

$$A = \alpha d\theta + \cdots \tag{30}$$

Here, (r, θ) are radial coordinates in the normal plane, α is the parameter which labels surface operators and takes values in $\mathfrak{t} = \mathrm{Lie}(\mathbb{T})$, the Lie algebra of the maximal torus $\mathbb{T} \subset G$, and the dots in (30) stand for less singular terms. More precisely, inequivalent choices of α are labeled by elements in $\mathbb{T} = \mathfrak{t}/\Lambda_{\mathrm{cochar}}$ since gauge transformations shift α by vectors in the cocharacter lattice $\Lambda_{\mathrm{cochar}}$ of G. For example, for $G = SU(2)$ we have $\mathbb{T} = U(1)$.

In the presence of a surface operator on $D \subset X$, supersymmetric field configurations in this theory are described by the instanton equations (25):

$$F_A^+ = 2\pi\alpha(\delta_D)_+ \tag{31}$$

perturbed by the term $2\pi\alpha(\delta_D)_+$, where $(\delta_D)_+$ denotes the self-dual part of the cohomology class that is Poincaré dual to the surface D. In the context of $SU(2)$ gauge theory, such surface operators were extensively used in the work of Kronheimer and Mrowka on minimal genus problems of embedded surfaces in 4-manifolds [46, 47].

According to the general rules outlined in the previous section, to a 4-manifold $X = \mathbf{R} \times Y$ and a surface operator on $D = \mathbf{R} \times K$ labeled by $e^{2\pi i\alpha} \in \mathbb{T}$ the Donaldson-Witten theory associates a vector space, the space of quantum ground states,

$$\mathscr{H}_{Y;K,\alpha} = HF_*^{\text{inst}}(Y; K, \alpha) \tag{32}$$

Just like the ordinary instanton Floer homology (27), it categorifies a Casson-like invariant,

$$\chi(\mathscr{H}_{Y;K,\alpha}) = \lambda_\alpha(Y; K) \tag{33}$$

which counts flat $SU(2)$ connections on a homology sphere Y with the prescribed singularity (30) along K.

In order to describe $\lambda_\alpha(Y; K)$ more explicitly, it is convenient to decompose Y as in (5) into a tubular neighborhood of the knot K, $Y_1 = N(K)$, and its complement, $Y_2 = Y \setminus N(K)$, glued along the common boundary $\Sigma \cong T^2$. As we already mentioned earlier, topological reduction of the Donaldson-Witten theory on Σ yields a topological A-model with the target space $\mathscr{M} = \mathscr{M}^G_{flat}$, the moduli space of flat connections on Σ:

$$\mathscr{M}^G_{flat} = \{\rho : \pi_1(\Sigma) \to G\}/\text{conj.} \tag{34}$$

For $\Sigma = T^2$ this moduli space is the quotient, $\mathscr{M}^G_{flat} = (\mathbb{T} \times \mathbb{T})/\mathscr{W}$, of two copies of the maximal torus by the Weyl group of G. In particular, for $G = SU(2)$ the corresponding moduli space $\mathscr{M}^G_{flat} \cong T^2/\mathbb{Z}_2$ is often called the "pillowcase". Similarly, each component in the decomposition $Y = Y_1 \cup_\Sigma Y_2$ defines an A-brane supported on a Lagrangian submanifold in $\mathscr{M}^G_{flat}$. If we denote Lagrangian submanifolds associated to Y_1 and Y_2, respectively, by $\mathscr{L}_\alpha$ and $\mathscr{L}_{Y\setminus K}$, then the invariant (33) is given by their intersection number (in the smooth part of $\mathscr{M}^G_{flat}$):

$$\lambda_\alpha(Y; K) = \#(\mathscr{L}_\alpha \cap \mathscr{L}_{Y\setminus K}) \tag{35}$$

Note, the Lagrangian brane supported on $\mathscr{L}_\alpha$ does not depend on K or Y, while the Lagrangian brane supported on $\mathscr{L}_{Y\setminus K}$ does not depend on α. Indeed, $\mathscr{L}_\alpha$ is simply the set of representations $\rho \in \mathscr{M}^G_{flat}$ taking the meridian of the knot K to a matrix of trace $\text{tr}(\rho_\mu) = 2\cos\pi\alpha$. Similarly, the Lagrangian brane supported on $\mathscr{L}_{Y\setminus K}$ corresponds to flat connections on $\Sigma = T^2$ which can be extended to flat connections on $Y \setminus K$. In other words, $\mathscr{L}_{Y\setminus K}$ is the image of $\mathscr{M}^G_{flat}(Y \setminus K)$ under the restriction map

$$r : \mathscr{M}^G_{flat}(Y \setminus K) \to \mathscr{M}^G_{flat}(T^2)$$

induced by the inclusion of the torus boundary of the knot complement, $T^2 \hookrightarrow Y \setminus K$.

To summarize, surface operators in the Donaldson-Witten theory lead to a variant of the instanton Floer homology, $\mathscr{H}_{Y;K,\alpha}$, whose Euler characteristic is a Casson-like invariant (35). This is precisely the definition of the knot invariant which was introduced and studied in [53, 9, 25] (see also [26, 45]). This invariant, sometimes called Casson-Lin invariant, is well-defined away from the roots of the Alexander polynomial of K and turns out to be equal to the linear combination of more familiar invariants, $\alpha \in [0, 1]$,

$$\lambda_\alpha(Y; K) = 4\lambda(Y) + \frac{1}{2}\sigma_\alpha(K) \tag{36}$$

where $\lambda(Y)$ is the Casson invariant of Y and $\sigma_\alpha(K) : U(1) \to \mathbb{Z}$ is the equivariant signature function (*a.k.a.* Levine-Tristram signature) of the knot K. Homology theory categorifying $\lambda_\alpha(Y; K)$ was constructed in [12] (see also [10, 11]) and, therefore, is expected to be the same as (32).

We remind that, for a knot K in a homology sphere Y, the normalized Alexander polynomial is defined as

$$\Delta(K; q) = \det\left(q^{1/2}\mathbf{V} - q^{-1/2}\mathbf{V}^T\right) \tag{37}$$

where $\mathbf{V}$ is the Seifert matrix of K and $q = e^{2\pi i\alpha}$. Note, that $\Delta(K; q) = \Delta(K; q^{-1})$. The equivariant signature $\sigma_\alpha(K)$ is defined as the signature of the Hermitian matrix

$$B_K(q) = (1 - q)\mathbf{V} + (1 - \overline{q})\mathbf{V}^T \tag{38}$$

The equivariant signature function changes its value only if $q = e^{2\pi i\alpha}$ is a root of the Alexander polynomial. It vanishes for α near 0 or 1,

$$\lim_{\alpha\to 0,1} \sigma_\alpha(K) = 0 \tag{39}$$

and equals the standard knot signature, $\sigma(K)$, for $\alpha = \frac{1}{2}$. In particular, for $Y = \mathbf{S}^3$ and $\alpha = \frac{1}{2}$ we get the original Lin's invariant [53] and the corresponding homology theory categorifying $\lambda_{\frac{1}{2}}(Y; K)$ was constructed—as symplectic Floer homology (24) of the braid representative of K—in [50].

3.2 Seiberg-Witten Theory

Now let us consider $\mathscr{N} = 2$ twisted gauge theory with Abelian gauge group $G = U(1)$ coupled to a single monopole field M. This theory localizes on the solutions to the Seiberg-Witten equations for Abelian monopoles [74]:

$$F_A^+ + i(\overline{M}M)_+ = 0 \tag{40}$$

$$\not{D}_A M = 0 \tag{41}$$

which follow from the $\mathcal{N} = 2$ topological gauge theory.[4] The partition function of this theory on a 4-manifold X with 2-observables included is a generating function of the Seiberg-Witten invariants, $SW_X(x)$, which "count" solutions to (40) and can be viewed as a function of $x \in \mathrm{Spin}^c(X)$,

$$SW_X : \mathrm{Spin}^c(X) \to \mathbb{Z}$$

To be more precise, the Seiberg-Witten invariants are defined as integrals over $\mathscr{M}_x$, the moduli space of solutions to the Seiberg-Witten equations (40),

$$SW_X(x) = \int_{\mathscr{M}_x} a_D^{d_x/2}$$

where $d_x = \frac{1}{4}(x^2 - 2\chi(X) - 3\sigma(X))$ is the virtual dimension of $\mathscr{M}_x$, and a_D is a 2-form which represents the first Chern class of the universal line bundle on the moduli space $\mathscr{M}_x$.

The space of quantum ground states in this theory is the Seiberg-Witten monopole homology,

$$\mathscr{H}_Y = HM_*(Y) \tag{44}$$

which is conjectured to be isomorphic to the Heegard Floer homology, see e.g. [48]:

$$HM_*(Y) \cong HF_*(Y) \tag{45}$$

In turn, the Heegard Floer homology $HF_*(Y)$—as well as its analog for knots, the knot Floer homology $HFK_*(K)$, that is closer to our interest—is defined as the symplectic Floer homology of certain Lagrangian submanifolds in the symmetric product space of the form [62, 64, 61],

$$\mathscr{M} = \mathrm{Sym}^k(\Sigma) \tag{46}$$

The symmetric product space and Lagrangian submanifolds in it naturally appear in the topological reduction of the Seiberg-Witten theory. Indeed, on $X = \mathbf{R}^2 \times \Sigma$ the

[4] Up to the finite group $H^1(X, \mathbb{Z}_2)$, the set of Spin^c structures on a 4-manifold X is parameterized by integral cohomology classes which reduce to $w_2(X)$ mod 2,

$$\mathrm{Spin}^c(X) = \{x \in H^2(X, \mathbb{Z}) \mid x \equiv w_2(X) \bmod 2\}$$

Given a Spin^c structure $x \in \mathrm{Spin}^c(X)$, let L be the corresponding Hermitian line bundle, and $S_L^{\pm}$ the corresponding spinor bundles. Then, the Seiberg-Witten monopole equations (40) are equations for a pair (A, M), where A is a unitary connection on L and M is a smooth section of S_L^+. In writing the equations (40) we used the Dirac operator, $\not{D}_A : S_L^+ \to S_L^-$, and a map

$$\Omega^0(S_L^+) \to \Omega^0(\mathrm{ad}_0 S_L^+) \tag{42}$$

$$M \mapsto i(\overline{M}M)_+ \tag{43}$$

where $\mathrm{ad}_0 S_L^+ \cong \Lambda_+^2$ is the subbundle of the adjoint bundle of S_L^+ consisting of the traceless skew-Hermitian endomorphisms, which can be identification with the space of self-dual 2-forms.

equations (40) reduce to the vortex equations in the Abelian Higgs model, and the moduli space of solutions to these equations, namely the moduli space of charge k vortices, is the symmetric product space (46), see [35]. As in the case of the Donaldson-Witten theory, the topological reduction of the Seiberg-Witten theory leads to the topological A-model[5] with $\mathscr{M}$ as the target space, and the corresponding category of branes in this case is the category of A-branes,

$$\mathscr{F}(\Sigma) = \mathbf{Fuk}(\mathscr{M}) \tag{47}$$

According to the general rules explained in the previous section, the Euler characteristic of the homology theory (44), (45) is given by the partition function of the Seiberg-Witten theory on $X = \mathbf{S}^1 \times Y$ (in the chamber $R \to \infty$):

$$Z_{SW}(Y) = \sum_{x \in \mathrm{Spin}^c(Y)} SW_Y(x) \tag{48}$$

If $b_1(Y) > 1$, then there are no wall-crossing phenomena and $Z_{SW}(Y)$ can be equivalently viewed as the partition function of the three-dimensional gauge theory on Y obtained by the dimensional reduction of the Seiberg-Witten theory. For a fairly general class of 3-manifolds Y, the partition function (48) is equal to the Casson invariant of Y, cf. (28):

$$Z_{SW}(Y) = \lambda(Y) \tag{49}$$

For instance, for 3-manifolds with $b_1(Y) > 1$ it follows e.g. from the general result of Meng and Taubes [58] that will be discussed in more detail below. On the other hand, for homology spheres the definition of the Seiberg-Witten invariants requires extra care. However, once this is done, one can show that (49) still holds for suitably defined $Z_{SW}(Y)$; see [52, 8, 59] for a mathematical proof and [4] for a physical argument based on the duality with Rozansky-Witten theory [65].

Surface Operators

As in the Donaldson-Witten theory, we can introduce surface operators by requiring the gauge field to have the singularity of the form (30). In the Seiberg-Witten theory, such surface operators are labeled by $e^{2\pi i\alpha} \in U(1)$. In the presence of a surface operator on $D \subset X$, supersymmetric field configurations are described by the perturbed Seiberg-Witten monopole equations, *cf.* [74, 71]:

$$F_A^+ + i(\overline{M}M)_+ = 2\pi\alpha(\delta_D)_+ \tag{50}$$

$$\not{D}_A M = 0 \tag{51}$$

As usual, in order to obtain a homological invariant of a knot K in a 3-manifold Y_0 one should consider the Hilbert space of the gauge theory on $X = \mathbf{R} \times Y_0$ with a surface operator on $D = \mathbf{R} \times K$. In the context of Seiberg-Witten theory, this gives a vector space $\mathscr{H}_{Y_0;K;x,\alpha}$. More generally, given a link L with ℓ components one

[5] In fact, this is true for any four-dimensional $\mathscr{N} = 2$ gauge theory with the same type of topological twist [3].

can introduce ℓ surface operators, each with its own parameter α_i, $i = 1, \ldots, \ell$. The corresponding Hilbert space is

$$\mathscr{H}_{Y_0;L;x_i,\alpha_i} = HM_*(Y; x_i, \alpha_i) \tag{52}$$

where $Y = Y_0 \backslash L$ is the link complement, and parameters α_i determine the boundary conditions on Y. Namely, the holonomy of the $U(1)$ gauge connection A along the meridian of the i-th link component should be equal to $e^{2\pi i \alpha_i}$. We will be mainly interested in the case where $Y_0 = \mathbf{S}^3$ and $Y = \mathbf{S}^3 \setminus L$ is the link complement. In this case, (52) gives $(\ell + 1)$-graded link homology.

We introduce the graded Euler characteristic of the homological invariant (52),

$$\tau_{\alpha_i}(Y; q_i) := \sum_{x \in H(Y)} \chi(HM_*(Y; x_i, \alpha_i)) \cdot q^x \tag{53}$$

which is a formal power series in $q_i^{\pm 1}$, where $q_i = e^{h_i}$ and h_i are the generators of a free Abelian group,

$$H(Y) := H_1(Y, \mathbb{Z})/\text{torsion} \cong \mathbb{Z}^{b_1(Y)}$$

In particular, when Y is a link complement, the group $H(Y) = H_1(Y, \mathbb{Z}) \cong \mathbb{Z}^\ell$ is generated by the meridians of the link components.

In general, $\tau_{\alpha_i}(Y; q_i)$ is a non-trivial function of q_i and α_i. It is equal to the partition function of the Seiberg-Witten theory on $X = \mathbf{S}^1 \times Y$ (in the chamber $R \to \infty$):

$$\tau_{\alpha_i}(Y; q_i) = \sum_{x \in H(Y)} SW_Y(x, \alpha_i) \cdot q^x \tag{54}$$

This function is an interesting generalization of the Reidemeister-Milnor torsion, on the one hand, and the equivariant knot signature, on the other. Indeed, since the Seiberg-Witten theory is the low-energy description of the Donaldson-Witten theory, we expect the relation to the equivariant knot signature. On the other hand, if α_i is near 0 or 1 for all $i = 1, \ldots, \ell$, as in (39), then the partition function $Z_{SW}(Y; x_i, \alpha_i) = \tau_{\alpha_i}(Y; q_i)$ becomes the ordinary partition function of the link complement Y studied by Meng and Taubes [58] who showed that it is equal to the Reidemeister-Milnor torsion. Hence,

$$\lim_{\alpha_i \to 0,1} \tau_{\alpha_i}(Y; q_i) = \tau(Y; q_i) \tag{55}$$

where $\tau(Y; q_i)$ is the ordinary Reidemeister-Milnor torsion of Y. In particular, for $b_1(Y) > 1$ we have $\tau(Y; q_i) = \Delta(L; q_i)$, so that in this limit the homological invariant (52) categorifies the multi-variable Alexander polynomial $\Delta(L; q_i)$ of the link L,

$$\sum_{x \in H(Y)} \chi(\mathscr{H}_{L;x}) \cdot q^x = \Delta(L; q) \tag{56}$$

This suggests to identify the $(\ell + 1)$-graded homology theory (52) with the link Floer homology [63],

$$\mathscr{H}_{L;x} = HFL_*(L; x) \tag{57}$$

In the case of knots, the relation to the Alexander polynomial $\Delta(K; q)$ is slightly more delicate, in part due to metric dependence and wall crossing. It turns out, however, that even though individual Seiberg-Witten invariants are different in the positive and negative chamber, the corresponding generating functions are both equal to the Milnor torsion [58], so that (55) still holds. Note, that specializing (55) further to $q_i = 1$, we recover (49). It would be interesting to study the invariant $\tau_\alpha(Y; q)$ further, in particular, its relation to the equivariant knot signature $\sigma_\alpha(K)$.

4 Surface Operators and Knot Homologies in $\mathscr{N} = 4$ Gauge Theory

Now, let us consider surface operators and knot homologies in the context of $\mathscr{N} = 4$ topological super-Yang-Mills theory in four dimensions. Specifically, we shall consider the GL twist of the theory [36], with surface operators labeled by regular semi-simple conjugacy classes [21]. As we shall explain below, this theory provides a natural framework for categorification of the $G_{\mathbf{C}}$ Casson invariant, which counts flat connections of the complexified gauge group $G_{\mathbf{C}}$.

The topological reduction of this theory leads to a $\mathscr{N} = 4$ sigma-model [3, 24, 36], whose target space is a hyper-Kahler manifold $\mathscr{M}_H(\Sigma, G)$, the moduli space of solutions to the Hitchin equations on Σ [27]:

$$F - \phi \wedge \phi = 0 \tag{58}$$

$$d_A\phi = 0, \quad d_A \star \phi = 0 \tag{59}$$

This twist of the $\mathscr{N} = 4$ super-Yang-Mills theory has a rich spectrum of supersymmetric surface operators. In particular, here we will be interested in the most basic type of surface operators, which correspond to the singular behavior of the gauge field A and the Higgs field ϕ of the form [21]:

$$A = \alpha d\theta + \cdots, \tag{60}$$

$$\phi = \beta \frac{dr}{r} - \gamma d\theta + \cdots \tag{61}$$

where $\alpha, \beta, \gamma \in \mathfrak{t}$, and the dots stand for the terms less singular at $r = 0$. For generic values of the parameters α, β, γ, (60) defines a surface operator associated with the regular semi-simple conjugacy class $\mathfrak{C} \in G_{\mathbf{C}}$.

According to the general rules explained in Sect. 2, this topological field theory associates a homological invariant $\mathscr{H}_Y$ to a closed 3-manifold Y and, more generally, a knot homology $\mathscr{H}_{Y;K}$ to a 3-manifold with a knot (link) K. These homologies can be computed as in (6) and (24) using the Heegard decomposition of Y as

well as the braid group action on branes. The branes in questions[6] are branes of type (A, B, A) with respect to the three complex structures (I, J, K) of the hyper-Kahler space $\mathscr{M}_H(\Sigma, G)$. We can use this fact and analyze the branes in different complex structures in order to gain a better understanding of the homological invariant $\mathscr{H}_{Y,K}$ as well as the $G_{\mathbf{C}}$ Casson invariant itself. For example, in complex structure I it corresponds to counting parabolic Higgs bundles, a fact that has already been used e.g. in [5] for studying the $SL(2, \mathbb{C})$ Casson invariant for Seifert fibered homology spheres.

Complex Structure J: Counting Flat Connections

The B-model in complex structure J is obtained, e.g. by setting the theta angle to zero, $\mathrm{Re}(\tau) = 0$, and choosing $t = i$ (where t is a complex parameter that labels a family of GL twists of the $\mathscr{N} = 4$ super-Yang-Mills [36]). In complex structure J, the moduli space $\mathscr{M}_H(\Sigma, G) \cong \mathscr{M}_{flat}^{G_{\mathbf{C}}}(\Sigma)$ is the space of complexified flat connections $\mathscr{A} = A + i\phi$, and the surface operator (60) creates a holonomy,

$$V = \mathrm{Hol}(\mathscr{A}),$$

which is conjugate to $\exp(-2\pi(\alpha - i\gamma))$. Furthermore, at $t = i$ the supersymmetry equations of the four-dimensional gauge theory are equivalent to the flatness equations, $d\mathscr{A} + \mathscr{A} \wedge \mathscr{A} = 0$, which explains why (from the viewpoint of complex structure J) the partition function of this theory on $X = \mathbf{S}^1 \times Y$ with a surface operator on $D = \mathbf{S}^1 \times K$ computes the $G_{\mathbf{C}}$ Casson invariant,

$$Z = \lambda_{G_{\mathbf{C}}}(Y; K)$$

The space of ground states, $\mathscr{H}_{Y;K}$, is a categorification of $\lambda_{G_{\mathbf{C}}}(Y; K)$. In general, both $\lambda_{G_{\mathbf{C}}}(Y; K)$ and $\mathscr{H}_{Y;K}$ depend on the holonomy V, which characterizes surface operators. However, if V is regular semi-simple, as we consider here, then $\lambda_{G_{\mathbf{C}}}(Y; K)$ and $\mathscr{H}_{Y;K}$ do not depend on a particular choice of V.

Complex Structure K

Since the four-dimensional topological gauge theory (even with surface operators) does not depend on the parameter t that labels different twists, we can take $t = 1$, which leads to the A-model on $\mathscr{M}_H(\Sigma, G)$ with symplectic structure ω_K. This theory computes the same $G_{\mathbf{C}}$ Casson invariant and its categorification, $\mathscr{H}_{Y;K}$, but via counting solutions to the following equations on Y [36]:

$$F - \phi \wedge \phi = \star\big(D\phi_0 - [A_0, \phi]\big) \tag{62}$$

$$\star\, D\phi = [\phi_0, \phi] + DA_0 \tag{63}$$

$$\star\, D \star \phi + [A_0, \phi_0] = 0 \tag{64}$$

rather than flat $G_{\mathbf{C}}$ connections. In particular, given a Heegard decomposition $Y = Y_1 \cup_\Sigma Y_2$, the space of solutions to (62) on Y_1 (resp. Y_2) defines a Lagrangian

[6] E.g. branes $\mathscr{B}_1$ and $\mathscr{B}_2$ associated with the Heegard decomposition $Y = Y_1 \cup_\Sigma Y_2$.

A-brane in $\mathscr{M}_H(\Sigma, G)$ with respect to ω_K. This allows to express $\mathscr{H}_{Y;K}$ as the space of open string states between the corresponding A-branes $\mathscr{B}_1$ and $\mathscr{B}_2$, *cf.* (6),

$$\mathscr{H}_{Y;K} = HF_*^{\text{symp}}(\mathscr{M}_H; \mathscr{B}_1, \mathscr{B}_2)$$

This alternative definition of the $G_{\mathbf{C}}$ Casson invariant and its categorification that follows from the twisted $\mathcal{N} = 4$ gauge theory can be useful, for instance, for understanding situations when the (A, B, A) branes $\mathscr{B}_1$ and $\mathscr{B}_2$ intersect at singular points in $\mathscr{M}_H$ or over higher-dimensional subvarieties.

Categorification of the $SL(2, \mathbb{C})$ Casson Invariant

Now, let us return to the complex structure J and, for simplicity, take the gauge group to be $G = SU(2)$. Furthermore, we shall consider an important example of the sphere with four punctures:

$$\Sigma = \mathbf{CP}^1 \setminus \{p_1, p_2, p_3, p_4\}$$

which in gauge theory corresponds to inserting four surface operators. In complex structure J, $\mathscr{M}_H(\Sigma, G)$ is the moduli space of flat $G_{\mathbf{C}} = SL(2, \mathbb{C})$ connections with fixed conjugacy class of the monodromy around each puncture. It can be identified with the space of conjugacy classes of monodromy representations

$$\mathscr{M}_H(\Sigma, G) \cong \{\rho : \pi_1(\Sigma) \to G_{\mathbf{C}} \mid \rho(\gamma_i) \in \mathfrak{C}_i\}/\sim$$

where the representations are restricted to take the simple loop γ_i around the i-th puncture into the conjugacy class $\mathfrak{C}_i \subset G_{\mathbf{C}}$.

Using the fact that $\pi_1(\Sigma)$ is free on three generators, we can explicitly describe the moduli space $\mathscr{M}_H(\Sigma, G)$ by introducing holonomies of the flat $SL(2, \mathbb{C})$ connection around each puncture,

$$V_i = \text{Hol}_{p_i}(\mathscr{A}), \quad i = 1, \ldots, 4 \tag{65}$$

where $V_1 V_2 V_3 V_4 = 1$ and each V_i is in a fixed conjugacy class. Following [32, 30, 33, 66, 28], we introduce the local monodromy data

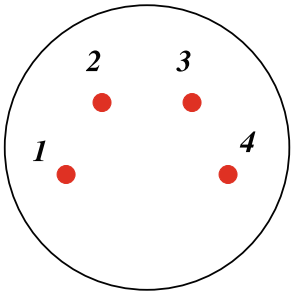


Fig. 6 Sphere with four punctures

$$a_i = \begin{cases} \mathrm{tr} V_i & i = 1, 2, 3 \\ \mathrm{tr}(V_3 V_2 V_1) & i = 4 \end{cases} \tag{66}$$

and

$$\theta_1 = a_1 a_4 + a_2 a_3 \tag{67}$$

$$\theta_2 = a_2 a_4 + a_1 a_3 \tag{68}$$

$$\theta_3 = a_3 a_4 + a_2 a_1$$

$$\theta_4 = a_1 a_2 a_3 a_4 + \sum_{i=1}^{4} a_i^2 - 4 \tag{69}$$

which determines the conjugacy classes of V_i. We also introduce the variables

$$x_1 = \mathrm{tr}(V_3 V_2) \tag{70}$$

$$x_2 = \mathrm{tr}(V_1 V_3) \tag{71}$$

$$x_3 = \mathrm{tr}(V_2 V_1) \tag{72}$$

which will be the coordinates on the moduli space $\mathscr{M}_H(\Sigma, G)$. Namely, the moduli space we are interested in is

$$\mathscr{M}_H(\Sigma, G) = \{(V_1, \ldots, V_4) \mid V_i \in \mathfrak{C}_i,\ V_1 V_2 V_3 V_4 = 1\}/G_{\mathbf{C}}$$

In terms of the variables (70), it can be explicitly described as the affine cubic

$$\mathscr{M}_H(\Sigma, G) = \{(x_1, x_2, x_3) \in \mathbb{C}^3 \mid f(x_i, \theta_m) = 0\} \tag{73}$$

where

$$f(x_i, \theta_m) = x_1 x_2 x_3 + \sum_{i=1}^{3} (x_i^2 - \theta_i x_i) + \theta_4 \tag{74}$$

Singularities in $\mathscr{M}_H$

For certain values of the monodromy data, the moduli space $\mathscr{M}_H$ becomes singular. It is important to understand the nature of the singularities and when they develop. In fact, as we shall see below, interesting examples of branes pass through such singularities.

The discriminant $\Delta(f)$ of the cubic (74) is a polynomial in a_i of total degree 16 [31]:

$$\Delta(a) = \left(\prod_{\epsilon_1 \epsilon_2 \epsilon_3 = 1} \left(a_4 + \sum \epsilon_i a_i \right) - \prod_{i=1}^{3} (a_i a_4 - a_j a_k) \right)^2 \prod_{i=1}^{4} (a_i^2 - 4) \tag{75}$$

where $\epsilon_i = \pm 1$. A special subfamily of cubics (74), which will play an important role in applications to knot invariants discussed below, corresponds to the case

where all monodromy parameters a_i are equal, $a_i = a$, $i = 1, 2, 3, 4$. In this case,

$$\theta_i = 2a^2, \quad i = 1, 2, 3 \tag{76}$$

$$\theta_4 = a^4 + 4a^2 - 4 \tag{77}$$

and it is easy to verify that $\Delta(a) = 0$. Specifically, for generic values of the parameter a, the moduli space $\mathscr{M}_H$ has three simple singularities of type A_1 (double points) at

$$(x_i, x_j, x_k) = (a^2 - 2, 2, 2) \tag{78}$$

These singularities correspond to reducible flat connections. For special values of a, the singularities can become worse and/or additional singularities can appear. For example, for $a^2 = 0$ a new singularity of type A_1 develops at the point $(x_1, x_2, x_3) = (-2, -2, -2)$. On the other hand, for $a^2 = 4$ the moduli space has a simple singularity of type D_4 at $(x_1, x_2, x_3) = (2, 2, 2)$.

Braid Group Action

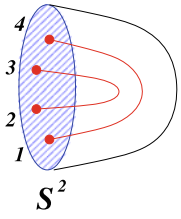
The mapping class group of Σ, which in the present case is the braid group Br_3, acts on the family of cubic surfaces (73) by polynomial automorphisms. In particular, one can verify that the generators σ_i, $i = 1, 2, 3$, represented as [32]:

$$\sigma_i \ : \ (x_i, x_j, x_k, \theta_i, \theta_j, \theta_k, \theta_4) \to (\theta_j - x_j - x_k x_i, x_i, x_k, \theta_j, \theta_i, \theta_k, \theta_4) \tag{79}$$

satisfy the relations $\sigma_i \sigma_j \sigma_i = \sigma_j \sigma_i \sigma_j$ and $\sigma_k = \sigma_i \sigma_j \sigma_i^{-1}$. Here and below we denote by (i, j, k) any cyclic permutation of $(1, 2, 3)$.

Examples

Let us consider examples of (A, B, A) branes that arise from knotted surface operators in $\mathbf{R} \times \mathbf{B}^3$, where $\mathbf{B}^3$ denotes a 3-dimensional ball. We consider surface operators which are extended along the $\mathbf{R}$ direction and which meet the boundary $\mathbf{S}^2 = \partial \mathbf{B}^3$ at four points. The simplest example of such brane is

brane $\widetilde{\mathscr{B}} =$ 

(80)

We shall denote this brane $\widetilde{\mathscr{B}}$ (or $\widetilde{\mathscr{B}}_{(14)(23)}$ if we wish to specify which pairs of points on $\mathbf{S}^2$ it connects). Since the brane (80) identifies the monodromies around the points 1 and 4 (resp. 2 and 3),

$$V_1 = V_4^{-1}, \qquad V_2 = V_3^{-1} \tag{81}$$

it can be explicitly described as a subvariety of $\mathscr{M}_H$ defined by

$$x_1 = \mathrm{tr}(V_3 V_2) = 2 \tag{82}$$

Of course, we also need to set $a_1 = a_4$ and $a_2 = a_3$, so that

$$\theta_1 = a_1^2 + a_2^2 \tag{83}$$
$$\theta_2 = \theta_3 = 2a_1 a_2 \tag{84}$$
$$\theta_4 = a_1^2 a_2^2 + 2a_1^2 + 2a_2^2 - 4 \tag{85}$$

Substituting (82) and (83) into the cubic equation $f(x_i, \theta_m) = 0$, we find that the brane (80) can be described as a degenerate quadric,

$$(x_2 + x_3 - a_1 a_2)^2 = 0 \tag{86}$$

One can also think of it as a set of two coincident branes on $x_2 + x_3 = a_1 a_2$. By acting on this brane with the elements of the braid group (79), we can construct other examples of (A, B, A) branes in $\mathscr{M}_H$. Furthermore, by closing the braid one can obtain homological invariants of knots (links) in $\mathbf{S}^3$ as spaces of open strings between two such branes. In the rest of this section, we consider a few explicit examples.

Unknot: One way to construct the unknot is to take surface operators which correspond to two branes of type (80), as shown on the figure below:

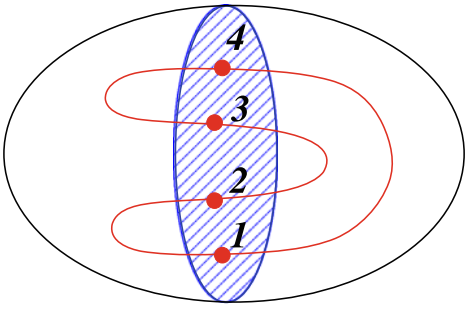


Fig. 7 Unknot in $\mathbf{S}^3$ can be represented as a union of two branes $\widetilde{\mathscr{B}}$

The two branes on this figure are branes $\widetilde{\mathscr{B}}_{(14)(23)}$ and $\widetilde{\mathscr{B}}_{(12)(34)}$. We already discussed the first brane: it is described by the conditions (82)–(86). Similarly, the brane $\widetilde{\mathscr{B}}_{(12)(34)}$ is given by $V_1 = V_2^{-1}$, which implies $V_3 = V_4^{-1}$,

$$x_3 = \mathrm{tr}(V_2 V_1) = 2 \tag{87}$$

and the corresponding conditions for θ_i, cf. (83). Altogether, the conditions describing these two branes imply that the local monodromy data should be identified,

$$a_1 = a_2 = a_3 = a_4 = a \tag{88}$$

This condition is very natural, of course, and will be relevant in all the examples where the resulting link has only one connected component, i.e. is actually a knot. Furthermore, for the unknot in Fig. 7 we have:

$$V_1 = V_2^{-1} = V_3 = V_4^{-1} \tag{89}$$

These equations describe the intersection points of branes $\widetilde{\mathscr{B}}_{(14)(23)}$ and $\widetilde{\mathscr{B}}_{(12)(34)}$. Using (82) and (87), it is easy to see that there is only one such point (of multiplicity 2):

$$(x_1, x_2, x_3) = (2, a^2 - 2, 2) \tag{90}$$

This is precisely one of the singular points (78) where the moduli space $\mathscr{M}_H$ has A_1 singularity (for generic values of a) due to reducible representations. Therefore, we conclude that the cohomology of the unknot, $\mathscr{H}^{sl(2)}_{\text{unknot}}$, is given by the space of open string states for two different branes intersecting at the A_1 singularity in $\mathscr{M}_H$. We point out that the values of x_i in (90) can be read off directly from Fig. 7. Indeed, $x_1 = 2$ simply follows from the fact that the combined monodromy around the points 2 and 3 is equal to the identity (similarly for $x_3 = 2$). In order to explain $x_2 = a^2 - 2$, it is convenient to introduce the eigenvalues $m^{\pm 1}$ of the monodromy matrix V_1. Of course, m is related to the local monodromy parameter a, namely $a = m + m^{-1}$. Moreover, since $V_1 = V_3$, we have

$$x_2 = \text{tr}(V_1 V_3) = m^2 + m^{-2} = a^2 - 2 \tag{91}$$

One can also construct the unknot using identical branes $\widetilde{\mathscr{B}}$ and the braid group action on one of them:
Here, the two parts of the unknot correspond to the branes $\widetilde{\mathscr{B}}$ and $\phi_{\sigma_1}(\widetilde{\mathscr{B}})$, where $\widetilde{\mathscr{B}}$ is the brane described in (80)–(86), and σ_1 denotes the generator of the braid group Br_3. Using the explicit form (79) of σ_1, we find that the brane $\phi_{\sigma_1}(\widetilde{\mathscr{B}})$ is supported on the line:

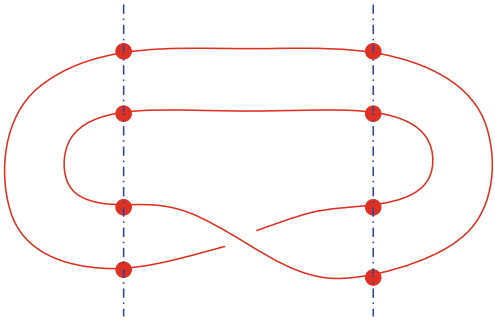


Fig. 8 Unknot as a union of two branes $\widetilde{\mathscr{B}}$ with a half-twist. Each vertical line represents a surface (topologically a 2-sphere) which divides $\mathbf{S}^3$ into two balls and meets the surface operator at four points

$$\phi_{\sigma_1}(\widetilde{\mathscr{B}}): \quad x_2 = 2 \tag{92}$$

Together with (82), this condition implies that the branes $\widetilde{\mathscr{B}}$ and $\phi_{\sigma_1}(\widetilde{\mathscr{B}})$ meet only at one point (of multiplicity 2):

$$(x_1, x_2, x_3) = (2, 2, a^2 - 2) \tag{93}$$

which is precisely one of the A_1 singularities (78) in the moduli space $\mathscr{M}_H$. This is in complete agreement with our previous analysis, where the same configuration of D-branes in $\mathscr{M}$ was found starting from the presentation of the unknot shown on Fig. 7. This agreement was expected, of course, since both presentations of the unknot on Figs. 7 and 8 are homotopy equivalent in $\mathbf{S}^3$. The second presentation (on Fig. 8) can be easily generalized to the trefoil knot and more general torus knots (links) of type $(2, k)$.

Trefoil Knot: The trefoil can be constructed by joining together the brane (80) and the brane obtained by action of three half-twists on $\widetilde{\mathscr{B}}$.

Starting with the equation (82) describing the brane $\widetilde{\mathscr{B}}$ and applying σ_1 three times, we find that the brane $\phi_{(\sigma_1)^3}(\widetilde{\mathscr{B}})$ is supported on the set of points

$$(x_1, x_2, x_3) = (4z - 2a^2z + 2a^2z^2 - 2z^3 + y(1 - z^2), -2 + 2a^2 - 2a^2z + yz + 2z^2, z) \tag{94}$$

where we assumed (88). Together with the equation $f(x_i) = 0$, this condition describes a subvariety in $\mathscr{M}_H$ of complex dimension 1. Using (82) and (94), it is easy to see that the branes $\widetilde{\mathscr{B}}$ and $\phi_{(\sigma_1)^3}(\widetilde{\mathscr{B}})$ intersect at two points. The first intersection point (of multiplicity 2) is precisely the singular point (93), as in the case of the unknot. The second intersection point (of multiplicity 4) is located at the regular point in $\mathscr{M}_H$,

$$(x_1, x_2, x_3) = (2, a^2 - 1, 1) \tag{95}$$

Combining the contributions from the two intersection points, we find that the cohomology for the trefoil knot has the following structure

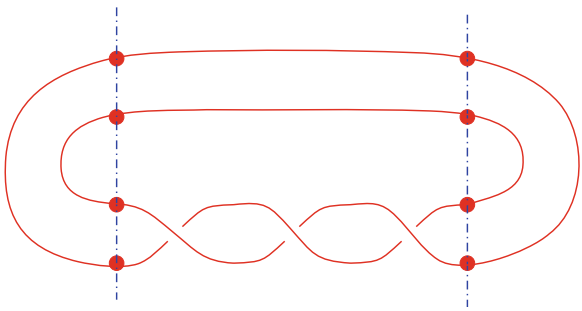


Fig. 9 The trefoil knot in $\mathbf{S}^3$ can be represented as a union of two branes $\widetilde{\mathscr{B}}$ with three half-twists

$$\mathscr{H}^{sl(2)}_{\text{trefoil}} = \mathscr{H}^{sl(2)}_{\text{unknot}} \oplus \mathscr{H}^{sl(2)}_{\times} \tag{96}$$

where $\mathscr{H}^{sl(2)}_{\text{unknot}}$ is the contribution from the first intersection point, and $\mathscr{H}^{sl(2)}_{\times}$ denotes the contribution from the new intersection point (95). Discarding the contribution of reducible connections, we find the *reduced* cohomology of the trefoil knot, which consists only of the term $\mathscr{H}^{sl(2)}_{\times}$,

$$\mathscr{H}^{sl(2)}_{\times} = \mathbb{C}^4 \tag{97}$$

Indeed, since $\mathscr{M}_H$ is smooth near the intersection point, the configuration of branes $\widetilde{\mathscr{B}}$ and $\phi_{(\sigma_1)^3}(\widetilde{\mathscr{B}})$ can be locally described (in complex structure J) as an intersection of two sets of B-branes in $\mathbf{C}^2$, such that each set is supported on a line in $\mathbf{C}^2$. Let us consider a slightly more general problem where two sets of B-branes in $\mathbf{C}^2$ contain n_1 and n_2 branes, respectively. We denote by $\mathscr{E}_1$ and $\mathscr{E}_2$ the corresponding sheaves, where $\mathscr{E}_1$ (and similarly $\mathscr{E}_2$) is defined by a module of the form $\mathbb{C}[x_1, x_2]/(x^{n_1})$. The space of open string states between two such B-branes is given by

$$\text{Ext}^*_{\mathbf{C}^2}(\mathscr{E}_1, \mathscr{E}_2) = \mathbb{C}^{n_1 n_2} \tag{98}$$

which, of course, is the expected result since in the present case open strings form a hypermultiplet transforming in (n_1, n_2) under $U(n_1) \times U(n_2)$. Setting $n_1 = n_2 = 2$ gives (97).

$(2, k)$ *Torus Knots*: A more general torus knot (link) $T_{2,k}$ can be represented as a union of two branes $\widetilde{\mathscr{B}}$ with k half-twists.

In order to describe the action of $(\sigma_1)^k$ on the brane (80), again we use (79). If the original brane $\widetilde{\mathscr{B}}$ is represented by a set of two coincident branes on the line (cf. (86)),

$$(x_1, x_2, x_3) = (2, y, a^2 - y) \tag{99}$$

the result of $(\sigma_1)^k$ action is a set of branes supported on a higher-degree curve

$$\phi_{(\sigma_1)^k}(\widetilde{\mathscr{B}}): \quad (x_1, x_2, x_3) = (P_k(y), P_{k-1}(y), a^2 - y) \tag{100}$$

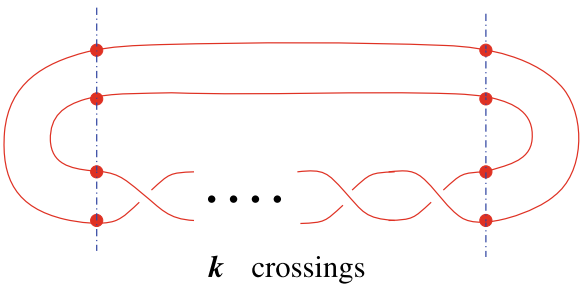


Fig. 10 The $(2, k)$ torus knot (link) in $\mathbf{S}^3$ can be represented as a union of two branes $\widetilde{\mathscr{B}}$ with k half-twists

where $\{P_i(y)\}_{i\geq -1}$ is a sequence of polynomials in y, such that $P_0(y) = 2$, $P_{-1}(y) = y$, and $P_i(y)$, $i > 1$ are determined by the recursion relation

$$P_i(y) = 2a^2 - (a^2 - y)P_{i-1}(y) - P_{i-2}(y)$$

For example, the first few polynomials $P_i(y)$ look like

$$P_1(y) = y \tag{101}$$
$$P_2(y) = -2 + 2a^2 - a^2y + y^2 \tag{102}$$
$$P_3(y) = 4a^2 - 2a^4 - 3y + 2a^2y + a^4y - 2a^2y^2 + y^3 \tag{103}$$
$$P_4(y) = 2 - 4a^4 + 2a^6 + 8a^2y - 4a^4y - a^6y - 4y^2 + 2a^2y^2 + 3a^4y^2 - 3a^2y^3 + y^4 \tag{104}$$
$$\vdots \tag{105}$$

For simplicity, let us focus on torus knots, which correspond to odd values of k (the case of k even, which corresponds to torus links, can be treated similarly). Then, it is easy to see that the brane $\phi_{(\sigma_1)^k}(\widetilde{\mathscr{B}})$ meets the brane (82) at $(k+1)/2$ points in $\mathscr{M}_H$. As in the case of the trefoil knot, one intersection point (of multiplicity 2) is the point (93) where $\mathscr{M}_H$ has A_1 singularity due to reducible connections. The other $(k-1)/2$ points (each of multiplicity 4) are generically located at regular points in $\mathscr{M}_H$; their precise location is determined by the explicit form of $P_i(y)$. Therefore, extending the earlier result (96), we find that cohomology $\mathscr{H}^{sl(2)}_{T_{2,k}}$ of the torus knot $T_{2,k}$ is isomorphic to a direct sum of $\mathscr{H}^{sl(2)}_{\text{unknot}}$ and $(k-1)/2$ copies of $\mathscr{H}^{sl(2)}_{\times} = \mathbb{C}^4$. As usual, it is convenient to remove the contribution of reducible solutions. If we denote by $\widetilde{\mathscr{H}}^{sl(2)}_K$ the "reduced" cohomology of K for the theory considered here, we can state our conclusion as

$$\dim \widetilde{\mathscr{H}}^{sl(2)}_{T_{2,k}} = 2(k-1) \tag{106}$$

In general, the cohomology $\widetilde{\mathscr{H}}^{sl(2)}_K$ categorifies a variant of the Casson invariant obtained by counting flat $SL(2,\mathbb{C})$ connections on the knot complement $\mathbf{S}^3 \setminus K$ with fixed conjugacy class of the holonomy around the meridian,

$$\chi(\widetilde{\mathscr{H}}^{sl(2)}_K) = 2\sigma(K) \tag{107}$$

We expect that, at least for a certain class of knots, $\sigma(K)$ is the ordinary knot signature. Notice, that for $(2,k)$ torus knots, we have $\sigma(T_{2,k}) = (k-1)$.

Finally, we note that one could obtain a different knot invariant (and, presumably, a different knot homology) by considering the image of the representation variety of the knot complement in the representation variety of the boundary torus, see e.g. [51]. Indeed, the boundary of the knot complement $Y \setminus K$ can be identified with T^2 in the usual way, and the inclusion $T^2 \hookrightarrow Y \setminus K$ induces the restriction map

$$r : \mathscr{M}_{flat}^{G_{\mathbf{C}}}(Y \setminus K) \to \mathscr{M}_{flat}^{G_{\mathbf{C}}}(T^2) \tag{108}$$

which maps a representation $\rho : \pi_1(Y \setminus K) \to G_{\mathbf{C}}$ to its restriction $\rho_{|T^2} : \pi_1(T^2) \to G_{\mathbf{C}}$. In general, $\mathscr{M}_{flat}^{G_{\mathbf{C}}}(Y \setminus K)$ is a branched cover of its image in $\mathscr{M}_{flat}^{G_{\mathbf{C}}}(T^2)$ under the restriction map (108). For example, if $G_{\mathbf{C}} = SL(2, \mathbb{C})$ and $Y = \mathbf{S}^3$ then, ignoring the multiplicity, the image of the representation variety $\mathscr{M}_{flat}^{G_{\mathbf{C}}}(\mathbf{S}^3 \setminus K)$ under the restriction map can be described as the zero locus[7] of the A-polynomial [13],

$$A(l, m) = 0 \tag{109}$$

where the complex variables l and m parameterize, respectively, the conjugacy classes of the holonomy of the flat $SL(2, \mathbb{C})$ connection along the longitude and the meridian of the knot. The A-polynomial of every knot has a factor $(l - 1)$ due to reducible representations. For example, the A-polynomial of a $(2, k)$ torus knot looks like

$$A(T_{2,k}) = (l - 1)(lm^{2k} + 1) \tag{110}$$

Notice, in this example, the part containing irreducible representations consists of a single curve, $lm^{2k} + 1 = 0$, of degree one in l. On the other hand, the $SL(2, \mathbb{C})$ representation variety of $T_{2,k}$ is a cover of this curve by $\frac{k-1}{2}$ distinct irreducible components which correspond to irreducible representations counted by $\mathscr{N} = 4$ topological gauge theory. Restricting the complex variables l and m to be on a unit circle, we obtain the image of the $SU(2)$ representation variety. For $(2, k)$ torus knots, the $SU(2)$ representation variety (again, ignoring reducible representations) is a disjoint union of $\frac{k-1}{2}$ nested open arcs [43, 6].

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Conformal Field Theory and Operator Algebras

Yasuyuki Kawahigashi*

Abstract We review recent progress in operator algebraic approach to conformal quantum field theory. Our emphasis is on use of representation theory in classification theory. This is based on a series of joint works with R. Longo.

1 Introduction

A mathematically rigorous approach to quantum field theory based on operator algebras is called an *algebraic quantum field theory*. It has a long history since pioneering works of Araki, Haag, Kastker. (See [26] for a general treatment of algebraic quantum field theory.) This theory works on Minkowski spaces on any spacetime dimension, and there have been some recent results on curved spacetimes or even noncommutative spacetimes. In the case of $1+1$-dimensional Minkowski space with higher spacetime symmetry, *conformal symmetry*, we have *conformal field theory* and there we have seen many new developments in the recent years, so we survey such results here. Our emphasis is on representation theoretic aspects of the theory and we make various comparison with another mathematically rigorous and more recent approach to conformal field theory, that is, theory of vertex operator algebras.

Roughly speaking, a mathematical study of quantum field theory is a study of Wightman fields, which are certain type of operator-valued distributions on a spacetime with covariance with respect to a given spacetime symmetry group. We have mathematically rigorous axioms for such Wightman fields, but they involve distributions and unbounded operators, so these cause various kinds of technical difficulty. In contrast, in the algebraic quantum field theory, our fundamental object is a *net*

Yasuyuki Kawahigashi
Department of Mathematical Sciences, University of Tokyo, Komaba, Tokyo, 153-8914, Japan, e-mail: yasuyuki@ms.u-tokyo.ac.jp

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of von Neumann algebras of bounded linear operators on a Hilbert space. (See [50–52] for general theory of von Neumann algebras.) Technical problems on definition domains of unbounded operators do not arise in this approach.

A basic idea is as follows. Suppose we have a Wightman field Φ on a spacetime. Fix a bounded region $\mathcal{O}$ in the space time and consider a test function φ with support contained in $\mathcal{O}$. Then the pairing $\langle \Phi, \varphi \rangle$ produces an (unbounded) operator. We have many Φ and φ for a fixed $\mathcal{O}$ and obtain many unbounded operators from such pairing. Then we consider a von Neumann algebra of *bounded* linear operators on this Hilbert space generated by these unbounded operators. (For example, if we have a self-adjoint unbounded operators, we consider its spectral projections which are obviously all bounded. In this way, we deal with only bounded operators.) This is regarded as a von Neumann algebra generated by *observables* in the spacetime region $\mathcal{O}$. A von Neumann algebra is an algebra of bounded linear operators which is closed under the adjoint operation and the strong operator topology. In this way, we have a family $\{\mathcal{A}(\mathcal{O})\}$ of von Neumann algebras on the same Hilbert space parameterized by spacetime regions. Since the spacetime regions make a net with respect to the inclusion order, we call such a family a net of von Neumann algebras. Now we forget Wightman fields and consider only a net of von Neumann algebras. We have some expected properties for such nets of von Neumann algebras from a physical consideration, and now we use these properties as *axioms*. So our mathematical object is a net of von Neumann algebras subject to certain set of axioms. Our mathematical aim is to study such nets of von Neumann algebras.

2 Conformal Quantum Field Theory

We first explain formulation of full conformal quantum field theory on the $1+1$-dimensional Minkowski space in algebraic quantum field theory. As a spacetime region $\mathcal{O}$ above, it is enough to consider only open rectangles $\mathcal{O}$ with edges parallel to $t = \pm x$ in $(1+1)$-dim Minkowski space. In this way, we get a family $\{\mathcal{A}(\mathcal{O})\}$ of operator algebras parameterized by spacetime regions $\mathcal{O}$ (rectangles). In order to realize conformal symmetry, we have to make a partial compactification of the $1+1$-dimensional Minkowski space. If two rectangles are spacelike separated, then we have no interactions between them even at the speed of light, so our axiom requires that the corresponding two von Neumann algebras commute with each other. This is the *locality axiom*. Since this is not our main object in this paper, we omit details of the other axioms. See [33] for full details.

Next we briefly explain that boundary conformal field theory can be handled within the same framework. Now we consider the half-space $\{(x,t) \mid x > 0\}$ in the $1+1$-dimensional Minkowski space and only rectangles $\mathcal{O}$ contained in this half-space. In this way, we have a similar net of von Neumann algebras $\{\mathcal{A}(\mathcal{O})\}$ parameterized with rectangles in the half-space. See [43] for full details of the axioms.

If we have a net of von Neumann algebras over the $1+1$-dimensional Minkowski space, we can *restrict* the net of von Neumann algebras to two *chiral* conformal field theories on the light cones $\{x = \pm t\}$. In this way, we have two nets of von Neumann algebras on the compactified S^1 as description of two *chiral* conformal field theories. Since this net is our main mathematical object in this article, we give a full set of axioms. (See [33] for details of this "restriction" procedure.)

Now our "spacetime" is S^1 and a "spacetime region" is an interval I, which means a non-empty, non-dense open connected subset of S^1. We have a family $\{\mathscr{A}(I)\}$ of von Neumann algebras on a fixed Hilbert space H. These von Neumann algebras are simple and such von Neumann algebras are called *factors*, so the family $\{\mathscr{A}(I)\}$ satisfying the axioms below is called a *net of factors* (or an *irreducible local conformal net of factors*, strictly speaking). Actually, the set of intervals on S^1 is not directed with respect to inclusions, so the terminology *net* is not mathematically appropriate, but is widely used.

1. (isotony) For intervals $I_1 \subset I_2$, we have $\mathscr{A}(I_1) \subset \mathscr{A}(I_2)$.
2. (locality) For intervals I_1, I_2 with $I_1 \cap I_2 = \varnothing$, we have $[\mathscr{A}(I_1), \mathscr{A}(I_2)] = 0$.
3. (Möbius covariance) There exists a strongly continuous unitary representation U of $PSL(2, \mathbb{R})$ on H satisfying $U(g)\mathscr{A}(I)U(g)^* = \mathscr{A}(gI)$ for any $g \in PSL(2, \mathbb{R})$ and any interval I.
4. (positivity of energy) The generator of the one-parameter rotation subgroup of U, called the *conformal Hamiltonian*, is positive.
5. (existence of the vacuum) There exists a unit U-invariant vector Ω in H, called the *vacuum vector*, and the von Neumann algebra $\bigvee_{I \in S^1} \mathscr{A}(I)$ generated by all $\mathscr{A}(I)$'s is $B(H)$.
6. (conformal covariance) There exists a projective unitary representation U of $\mathrm{Diff}(S^1)$ on H extending the unitary representation of $PSL(2, \mathbb{R})$ such that for all intervals I, we have

$$U(g)\mathscr{A}(I)U(g)^* = \mathscr{A}(gI), \quad g \in \mathrm{Diff}(S^1),$$
$$U(g)AU(g)^* = A, \quad A \in \mathscr{A}(I),\ g \in \mathrm{Diff}(I'),$$

   where $\mathrm{Diff}(S^1)$ is the group of orientation-preserving diffeomorphisms of S^1 and $\mathrm{Diff}(I')$ is the group of diffeomorphisms g of S^1 with $g(t) = t$ for all $t \in I$.

The isotony axiom is natural because we have more test functions (or more observables) for a larger interval. The locality axiom takes this simple form on S^1. The choice of the spacetime symmetry is not unique, and we can use the Poincaré symmetry on the Minkowski space or the Möbius covariance on S^1, for example, but in the *conformal* field theory, we use *conformal* symmetry, which means diffeomorphism covariance as above. This set of axioms imply various nice conditions such as the Reeh-Schlieder property, the Bisognano-Wichmann property and the Haag duality. See [32] and references there for details.

In the usual situation, all the von Neumann algebras $\mathscr{A}(I)$ are isomorphic to the so-called Araki-Woods type III_1 factor for all nets $\mathscr{A}$ and all intervals I. So each von Neumann algebra does not contain any information about the conformal field theory, but it is the relative position of the von Neumann algebras in

the family that encodes the physical information of the theory. (It is similar to subfactor theory of Jones where we study a relative position of one factor in another.)

At the end of this section, we compare our formulation of conformal quantum field theory with another mathematically rigorous approach, theory of vertex operator algebras. A vertex operator algebra is an algebraic axiomatization of Wightman fields on S^1, called vertex operators. If we have an operator valued distribution on S^1, its Fourier expansion should give countably many (possibly unbounded) operators as the Fourier coefficients. Under the so-called state-field correspondence, any vector in the space of "states" should give an operator-valued distribution, a quantum "field", and its Fourier expansion gives countably many operators. In this way, one vector should give countably many operators on the space of these vectors. In other words, for two vectors v, w we have countably many binary operations $v_{(n)}w$, $n \in \mathbb{Z}$, the action of the n-th operator given by v on w. An axiomatization of this idea gives a notion of *vertex operator algebra*. (See [20] for a precise definition. There is a slightly weaker notion of a *vertex algebra*. See [31] for its precise definition and related results.) In theory of vertex operator algebra, one considers a vector space of states without an inner product and even when we have a positive definite inner product, one considers this vector space without completion. Here in comparison to nets of factors, we are interested in the case where we have positive definite inner products on the spaces of states. We say that such a vertex operator algebra is *unitary*.

Both of one (unitary) vertex operator algebra and one net of factors should describe one chiral conformal field theory. So unitary vertex operator algebras and nets of factors should be in a bijective correspondence, at least under some "nice" additional conditions, but no general theorems have been known for such a correspondence, though there is a recent progress due to S. Carpi and M. Weiner. However, if we have one construction or an idea on one side, we can often "translate" it to the other side, though it can be highly non-trivial from a technical viewpoint. Fundamental sources of constructions for vertex operator algebras are affine Kac-Moody algebras and integral lattices. The corresponding constructions for nets of factors have been done by A. Wassermann [54] and his students, and Dong-Xu [12], respectively, after the initial construction of Buchholz-Mack-Todorov [7]. If we have examples with some nice properties, we can often construct new examples from them, and as such methods of constructions of vertex operator algebras, we have simple current extensions, the coset construction, and the orbifold construction. The simple current extensions for nets of factors are simply crossed products by DHR-automorphisms and easy to realize. (See the next section for a notion of DHR-endomorphisms.) The coset and orbifold constructions for nets of factors have been studied in detail by F. Xu [58, 56, 59].

For nets of factors, we have introduced a new construction of examples in [32] based on Longo's notion of Q-systems [41]. Further examples have been constructed by Xu [62] with this method. This can be translated to the setting of vertex operator algebras, as we will see in this article later.

3 Representation Theory

An important tool to study nets of factors is a representation theory. For a net of factors $\{\mathscr{A}(I)\}$, all the algebras $\mathscr{A}(I)$ act on the initial Hilbert space H from the beginning, but we also consider their representations on another Hilbert space, that is, a family $\{\pi_I\}$ of representations $\pi_I : \mathscr{A}(I) \to B(K)$, where K is another Hilbert space, common for all I. For $I_1 \subset I_2$, we must have that the restriction of π_{I_2} on $\mathscr{A}(I_1)$ is equal to π_{I_1}. The representation on the initial Hilbert space is called the *vacuum representation* and plays a role of a trivial representation. We also have to take care of the spacetime symmetry group when we consider a representation, but this part is often automatic (see [24]), so we now ignore it for simplicity. See [24] for a more detailed treatment. Note that a representation of a net of factors is a counterpart of a module over a vertex operator algebra.

Notions of irreducibility and a direct sum for such representations are easy to formulate. Non-trivial notions are dimensions and tensor products. Each representation $\{\pi_I\}$ is in a bijective correspondence to a certain *endomorphism* λ of an infinite dimensional operator algebra, called a Doplicher-Haag-Roberts (DHR) endomorphism [15, 16, 18, 19], and we can restrict λ to a single factor $\mathscr{A}(I)$ for an arbitrarily but fixed interval I. Then $\lambda(\mathscr{A}(I)) \subset \mathscr{A}(I)$ is a subfactor and we have its Jones index [30]. (See [17, 46, 48] for general theory of subfactors.) The square root of this Jones index plays the role of the *dimension* of the representation [39, 40]. In algebraic quantum field theory, such a dimension was called a *statistical dimension*, and it is analogous to a quantum dimension in the theory of quantum groups. It is a positive real numbers in the interval $[1, \infty]$. We can also compose endomorphisms and this composition gives the correct notion of *tensor products*. We then get a *braided* tensor category as in [18, 19].

In representation theory of a vertex operator algebra (and also a quantum group), it sometimes happens that we have only finitely many irreducible representations. Such finiteness is often called *rationality*, possibly with some extra assumptions on some finite dimensionality. This also plays an important role in theory of quantum invariants in low dimensional topology. In [36], we have introduced an operator algebraic condition for such rationality for nets of factors as follows and we called it *complete rationality*. We split the circle into four intervals I_1, I_2, I_3, I_4 in this order, say, counterclockwise. Then complete rationality is given by the finiteness of the Jones index for a subfactor $\mathscr{A}(I_1) \vee \mathscr{A}(I_3) \subset (\mathscr{A}(I_2) \vee \mathscr{A}(I_4))'$ where $'$ means the commutant, together with the *split property*. The split property is known to hold if the *vacuum character*, $\sum_{n=0}(\dim H_n)q^n$, is convergent for $|q| < 1$ by [11], so it usually holds and is easy to verify. (Here $H = \bigoplus_{n=0}^{\infty} H_n$ is the eigenspace decomposition of the original Hilbert space for the positive generator of the rotation group. So this convergence property can be verified simply by looking at the Hilbert space, not the von Neumann algebras.) In the original definition of complete rationality in [36], we required another condition called strong additivity, but it was proved to be redundant by Longo-Xu [44]. We have proved in [36] that this complete rationality implies that we have a *modular* tensor category as a representation category of $\{\mathscr{A}(I)\}$. A modular tensor category produces a 3-dimensional topolog-

ical quantum field theory. (See [53] for general theory of topological quantum field theory.) The $SU(N)_k$-net of Wassermann has been shown to be completely rational by [57].

We now introduce an important notion of *α-induction*. For an inclusion of nets of factors, $\mathscr{A}(I) \subset \mathscr{B}(I)$, we have an induction procedure analogous to the group representation. So from a representation of the smaller net $\mathscr{A}$, we would like to construct a representation of the larger net $\mathscr{B}$, but what we actually obtain is not a genuine representation of the larger net $\mathscr{B}$ in general, and is something weaker called *solitonic*. This induction procedure is called the α-induction and depends a choice of braiding, so we write α^+ and α^-. This was first defined in Longo-Rehren [42] and studied in detail in Xu [55]. Then Böckenhauer-Evans [1–3] made a further study, and [4, 5] unified this study with Ocneanu's graphical method [47]. The intersection of the irreducible endomorphisms appearing in the images of α^+-induction and α^--induction gives the true representation category of $\{\mathscr{B}(I)\}$ if $\mathscr{A}$ is completely rational by [4, 36].

This α-induction opens an important and new connection with theory of *modular invariants*. A modular tensor category produces a unitary representation π of $SL(2,\mathbb{Z})$ through its braiding as in [49], and its dimension is the number of irreducible objects. So a completely rational net of factors produces such a unitary representation. (Note that our representation of $SL(2,\mathbb{Z})$ comes from the braiding structure, not from the action of this group on the characters through change of variables $\tau \mapsto \frac{a\tau+b}{c\tau+d}$, though in all the "nice" known examples, these two representations coincide. See [34] for a discussion on this matter.)

It has been proved in [4] that the matrix $(Z_{\lambda,\mu})$ defined by

$$Z_{\lambda,\mu} = \dim \mathrm{Hom}(\alpha^+_\lambda, \alpha^-_\mu)$$

is in the commutant of the representation π, using Ocneanu's graphical calculus [47]. Such a matrix Z is called a *modular invariant*, and we have only finitely many such Z for a given π. For any completely rational net $\{\mathscr{A}(I)\}$, any extension $\{\mathscr{B}(I) \supset \mathscr{A}(I)\}$ produces such Z. Matrices Z are certainly much easier to classify than extensions and this is a source of classification theory in the next section.

4 Classification Theory

For a net of factors, we can naturally define a *central charge* and it is well-known to take discrete values $1 - 6/m(m+1)$, $m = 3, 4, 5, \ldots$, below 1 and all values in $[1, \infty)$ by [21, 22]. We have the *Virasoro net* $\{\mathrm{Vir}_c(I)\}$ for each such c and it is the operator algebraic counterpart of the Virasoro vertex operator algebra with the same c. Any net of factors $\{\mathscr{A}(I)\}$ with central charge c is an extension of the Virasoro net with the same central charge and it is automatically completely rational if $c < 1$, as shown in [32]. So we can apply the above theory and we get the following complete classification list for the case $c < 1$ as in [32].

1. The Virasoro nets $\{\mathrm{Vir}_c(I)\}$ with $c < 1$.
2. The simple current extensions of the Virasoro nets with index 2.
3. Four exceptionals at $c = 21/22, 25/26, 144/145, 154/155$.

The unitary representations of $SL(2,\mathbb{Z})$ for the Virasoro nets are the well-known ones, and all the modular invariants for these have been classified by [8]. Our result shows that each of the so-called type I modular invariants in the classification list of [8] corresponds to a net of factors uniquely. They are labeled with pairs of A-D_{2n}-$E_{6,8}$ Dynkin diagrams with Coxeter numbers differing by 1. Three in (3) of the above list have been identified with coset models, but the remaining one does not seem to be related to any other known constructions. This is constructed with "extension by Q-system". Xu [62] recently applied this construction to many other coset models and obtained infinitely many new examples based on [61], called *mirror extensions*. Classification for the case $c = 1$ has been also done under some extra assumption [9, 60].

This classification theorem also implies a classification of certain types of vertex operator algebras as follows.

Let V be a (rational) vertex operator algebra and W_i be its irreducible modules. We would like to classify all vertex operator algebras arising from putting a vertex operator algebra structure on $\bigoplus_i n_i W_i$ and using the same Virasoro element as V, where n_i is multiplicity and $W_0 = V$, $n_0 = 1$. From a viewpoint of tensor category, this classification problem of extensions of a vertex operator algebras is the "same" as the classification problem of extensions of a completely rational net of factors, as shown in [28, 38].

So the above classification theorem of local conformal nets implies a classification theorem of extensions of the Virasoro vertex operator algebras with $c < 1$ as above, and we obtain the same classification list. That is, besides the Virasoro vertex operator algebras themselves, we have their simple current extensions, and four exceptionals at $c = 21/22, 25/26, 144/145, 154/155$. With the usual notation of $L(c,h)$ for a module with central charge c and conformal weight h of the Virasoro vertex operator algebras with $c < 1$, the four exceptionals are listed as follows.

1. $L(21/22,0) \oplus L(21/22,8)$. It has 15 irreducible representations and has two coset realizations, from $SU(9)_2 \subset (E_8)_2$ and $(E_8)_3 \subset (E_8)_2 \otimes (E_8)_1$.
2. $L(25/26,0) \oplus L(25/26,10)$. It has 18 irreducible representations and has a coset realization from $SU(2)_{11} \subset SO(5)_1 \otimes SU(2)_1$.
3. $L(144/145,0) \oplus L(144/145,24) \oplus L(144/145,78) \oplus L(144/145,189)$. It has 28 irreducible representations and no coset realization has been known.
4. $L(154/155,0) \oplus L(154/155,26) \oplus L(154/155,84) \oplus L(154/155,203)$. It has 30 irreducible representations and has a coset realization from $SU(2)_{29} \subset (G_2)_1 \otimes SU(2)_1$.

Note that it is not obvious that the representation category of the Virasoro net Vir_c and the representation category of the Virasoro vertex operator algebra $L(c,0)$ are isomorphic, but as long as the two are braided tensor category and have the same S- and T-matrices, the arguments in [32] work, so we obtain the above classification result for vertex operator algebras.

Using the above results and more techniques, we can also completely classify full conformal field theories within the framework algebraic quantum field theory for the case $c < 1$. Full conformal field theories are given as certain nets of factors on $1+1$-dimensional Minkowski space. Under natural symmetry and maximality conditions, those with $c < 1$ are completely labeled with the pairs of A-D-E Dynkin diagrams with the difference of their Coxeter numbers equal to 1, as shown in [33]. We now naturally have D_{2n+1}, E_7 as labels, unlike in the chiral case. The main difficulty in this work lies in proving uniqueness of the structure for each modular invariant in the Cappelli-Itzykson-Zuber list [8]. This is done through 2-cohomology vanishing for certain tensor categories. in the spirit of [29].

Furthermore, using the above results and more techniques we can also completely classify boundary conformal field theories for the case $c < 1$. Boundary conformal field theories are given as certain nets of factors on a $1 + 1$-dimensional Minkowski half-space. Under a natural maximality condition, these with $c < 1$ are now completely labeled with the pairs of A-D-E Dynkin diagrams with distinguished vertices having the difference of their Coxeter numbers equal to 1, as shown in [37] based on a general theory in [43]. The "chiral fields" in a boundary conformal field theory should produce a net of factors on the boundary (which is compactified to S^1) as in the operator algebraic approach. Then a general boundary conformal field theory restricts to this boundary to produce a *non-local* extension of this *chiral* conformal field theory on the boundary.

5 Moonshine Conjecture

The Moonshine conjecture, formulated by Conway-Norton [10], is about mysterious relations between finite simple groups and modular functions, since an observation due to McKay.

Today the classification of all finite simple groups is complete and the classification list contains 26 sporadic groups in addition to several infinite series. The largest group among the 26 sporadic groups is called the *Monster* group and its order is about 8×10^{53} ([23]).

One the one hand, the non-trivial irreducible representation of the Monster having the smallest dimension is 196883 dimensional. On the other hand, the following function, called *j-function*, has been classically studied in algebra.

$$j(\tau) = q^{-1} + 744 + 196884q + 21493760q^2 + 864299970q^3 + \cdots$$

For $q = \exp(2\pi i\tau)$, $\mathrm{Im}\,\tau > 0$, we have modular invariance property, $j(\tau) = j(\frac{a\tau+b}{c\tau+d})$ for $\left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right) \in SL(2,\mathbb{Z})$, and this is the only function, up to the constant term, satisfying this property and starting with q^{-1},

McKay noticed $196884 = 196883 + 1$, and similar simple relations for other coefficients of the j-function and dimensions of irreducible representations of the Monster group turned out to be true. Then Conway-Norton [10] formulated the

Moonshine conjecture roughly as follows, which has been now proved by Borcherds [6] in 1992.

1. We have a "natural" infinite dimensional graded vector space $V = \bigoplus_{n=0}^{\infty} V_n$ with some algebraic structure having a Monster action preserving the grading and each V_n is finite dimensional.
2. For any element g in the Monster, the power series $\sum_{n=0}^{\infty}(\mathrm{Tr}\, g|_{V_n})q^{n-1}$ is a special function called a *Hauptmodul* for some discrete subgroup of $SL(2,\mathbb{R})$. When g is the identity element, the series is the j-function minus constant term 744.

For the part (1) of this conjecture, Frenkel-Lepowsky-Meurman [20] gave a precise definition of "some algebraic structure" as a *vertex operator algebra* and constructed a particular example V, which is now called the *Moonshine vertex operator algebras* and denoted by $V^\natural$.

The construction roughly goes as follows. In dimension 24, we have an exceptional lattice Λ called the *Leech lattice*. Then there is a general construction of a vertex operator algebra from a certain lattice, and the one for the Leech lattice gives something very close to our final object $V^\natural$. Then we take a fixed point algebra under a natural action of $\mathbb{Z}/2\mathbb{Z}$ arising from the lattice symmetry, and then make a simple current extension of order 2. The resulting vertex operator algebra is the Moonshine vertex operator algebra $V^\natural$. (The final step is called a twisted orbifold construction.) The series $\sum_{n=0}^{\infty}(\dim V_n^\natural)q^{n-1}$ is indeed the j-function minus constant term 744.

Miyamoto [45] has a new realization of $V^\natural$ as an extension of a tensor power of the Virasoro vertex operator algebra with $c = 1/2$, $L(1/2,0)^{\otimes 48}$ (based on Dong-Mason-Zhu [13]). This kind of extension of a Virasoro tensor power is called a *framed vertex operator algebra* as in [14].

We have given an operator algebraic counterpart of such a construction in [35].

We realize a Leech lattice net of factors on S^1 as an extension of $\mathrm{Vir}_{1/2}{}^{\otimes 48}$ using certain $\mathbb{Z}_4$-code. Then we can perform the twisted orbifold construction in the operator algebraic sense to obtain a net of factors, the *Moonshine net* $\mathscr{A}^\natural$. Theory of α-induction is used for obtaining various decompositions. We then get a Miyamoto-type description of this construction, as an operator algebraic counterpart of the framed vertex operator algebras. We then have the following properties.

1. $c = 24$.
2. The representation theory is trivial.
3. The automorphism group is the Monster.
4. The Hauptmodul property (as above).

Outline of the proof of these four properties is as follows.

It is immediate to get $c = 24$. We can show complete rationality passes to an extension (and an orbifold) in general with control over the size of the representation category, using the Jones index. With this, we obtain (2) very easily. Such a net is called *holomorphic*. Property (3) is the most difficult part. For the Virasoro VOA $L(1/2,0)$, the vertex operator is indeed a well-behaved Wightman field and smeared fields produce the Virasoro net $\mathrm{Vir}_{1/2}$. Using this property and the fact that

$\bigcup_g g(L(1/2,0)^{\otimes 48})$ for all $g \in \mathrm{Aut}(V^\natural)$ generate the entire Moonshine VOA $V^\natural$, we can prove that the automorphism group as a vertex operator algebra and the automorphism group as a net of factors are indeed the same. Then (4) is now a trivial corollary of the Borcherds theorem [6].

We note that the Baby Monster, the second largest among the 26 sporadic finite simple groups, can be treated similarly with Höhn's construction of the shorter Moonshine super vertex operator algebra.

Still, these examples are treated with various tricks case by case. We expect a bijective correspondence between vertex operator algebras and nets of factors on S^1 under some nice conditions. On the side of vertex operator algebras, the most natural candidate for such a "nice" condition is the C_2-finiteness condition of Zhu [63] (with unitarity). On the operator algebraic side, our complete rationality in [36] seems to be such a "nice" condition, but the actual relations between the two notions are not clear at this moment. The essential condition for complete rationality is the finiteness of the Jones index arising from four intervals on the circle, and this finiteness somehow has formal similarity to the finiteness appearing in the definition of the C_2-finiteness.

At the end, we list some open problems. The operator algebraic approach has an advantage in control of representation theory, but is behind of theory of vertex operator algebras in the theory of characters.

For a net of factors, we can naturally define a notion of a character for each representation. But even convergence of these characters have not been proved in general, and the modular invariance property, the counterpart of Zhu's result [63], is unknown, though we certainly expect it to be true. We also expect the Verlinde identity holds, which has been proved in the context of vertex operator algebras recently by Huang [27]. We would need an S-matrix version of the spin-statistics theorem [25] for nets of factors.

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Diffusion and Mixing in Fluid Flow: A Review

Alexander Kiselev

Abstract This note is a review of a series of results on the interaction between diffusion and fluid flow that have been presented by the author at the International Congress in Mathematical Physics in Rio, 2006. The main object of study is the enhancement of diffusive mixing by a fast incompressible flow. Due to its physical relevance, the subject has been studied in detail from different angles. Here, we describe some of the recent work which combines PDE, functional analysis and dynamical systems theory by trying to establish links between diffusion enhancement and mixing properties inherent to the dynamical system generated by the flow. The proofs are based on a general criterion for the decay of the semigroup generated by an operator of the form $\Gamma + iAL$ with a negative unbounded self-adjoint operator Γ, a self-adjoint operator L, and parameter $A \gg 1$. In particular, they employ the RAGE theorem describing evolution of a quantum state belonging to the continuous spectral subspace of the Hamiltonian (related to a classical theorem of Wiener on Fourier transforms of measures).

1 Introduction

Let M be a smooth compact d-dimensional Riemannian manifold. The main subject of this paper is the effect of a strong incompressible flow on diffusion on M. Namely, we consider solutions of the passive scalar equation

$$\varphi_t^A(x,t) + Au \cdot \nabla \varphi^A(x,t) - \Delta \varphi^A(x,t) = 0, \quad \varphi^A(x,0) = \varphi_0(x). \tag{1}$$

Here Δ is the Laplace-Beltrami operator on M, u is a divergence free vector field, ∇ is the covariant derivative, and $A \in \mathbb{R}$ is a parameter regulating the strength of

Alexander Kiselev
Department of Mathematics, University of Wisconsin, Madison, WI 53706, USA, e-mail: kiselev@math.wisc.edu

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the flow. We are interested in the behavior of solutions of (1) for $A \gg 1$ at a fixed time $\tau > 0$.

It is well known that as time tends to infinity, the solution $\varphi^A(x,t)$ will tend to its average,

$$\overline{\varphi} \equiv \frac{1}{|M|}\int\limits_M \varphi^A(x,t)\,d\mu \frac{1}{|M|}\int\limits_M \varphi_0(x)\,d\mu,$$

with $|M|$ being the volume of M. We would like to understand how the speed of convergence to the average depends on the properties of the flow and determine which flows are efficient in enhancing the relaxation process.

The question of the influence of advection on diffusion is very natural and physically relevant, and the subject has a long history. The passive scalar model is one of the most studied PDEs in both mathematical and physical literature. One important direction of research focused on homogenization, where in a long time–large propagation distance limit the solution of a passive advection-diffusion equation converges to a solution of an effective diffusion equation. Then one is interested in the dependence of the diffusion coefficient on the strength of the fluid flow. We refer to [24] for more details and references. The main difference with the present work is that here we are interested in the flow effect in a finite time without the long time limit.

On the other hand, the Freidlin-Wentzell theory [13–16] studies (1) in $\mathbb{R}^2$ and, for a class of Hamiltonian flows, proves the convergence of solutions as $A \to \infty$ to solutions of an effective diffusion equation on the Reeb graph of the Hamiltonian. The graph, essentially, is obtained by identifying all points on any streamline. The conditions on the flows for which the procedure can be carried out are given in terms of certain non-degeneracy and growth assumptions on the stream function. The Freidlin-Wentzell method does not apply, in particular, to ergodic flows or in odd dimensions.

Perhaps the closest to our setting is the work of Kifer and more recently a result of Berestycki, Hamel and Nadirashvili. Kifer's work (see [17–20] where further references can be found) employs probabilistic methods and is focused, in particular, on the estimates of the principal eigenvalue (and, in some special situations, other eigenvalues) of the operator $-\epsilon\Delta + u\cdot\nabla$ when ϵ is small, mainly in the case of the Dirichlet boundary conditions. In particular, the asymptotic behavior of the principal eigenvalue λ_0^ϵ and the corresponding positive eigenfunction φ_0^ϵ for small ϵ has been described in the case where the operator $u\cdot\nabla$ has a discrete spectrum and sufficiently smooth eigenfunctions. It is well known that the principal eigenvalue determines the asymptotic rate of decay of the solutions of the initial value problem, namely

$$\lim_{t\to\infty} t^{-1}\log\|\varphi^\epsilon(x,t)\|_{L^2} = -\lambda_0^\epsilon \tag{2}$$

(see e.g. [18]). In a related recent work [2], Berestycki, Hamel and Nadirashvili utilize PDE methods to prove a sharp result on the behavior of the principal eigenvalue λ_A of the operator $-\Delta + Au\cdot\nabla$ defined on a bounded domain $\Omega \subset \mathbb{R}^d$ with the Dirichlet boundary conditions. The main conclusion is that λ_A stays bounded as

$A \to \infty$ if and only if u has a first integral w in $H_0^1(\Omega)$ (that is, $u \cdot \nabla w = 0$). An elegant variational principle determining the limit of λ_A as $A \to \infty$ is also proved. In addition, [2] provides a direct link between the behavior of the principal eigenvalue and the dynamics which is more robust than (2): it is shown that $\|\varphi^A(\cdot, 1)\|_{L^2(\Omega)}$ can be made arbitrarily small for any initial datum by increasing A if and only if $\lambda_A \to \infty$ as $A \to \infty$ (and, therefore, if and only if the flow u does not have a first integral in $H_0^1(\Omega)$). We should mention that there are many earlier works providing variational characterization of the principal eigenvalues, and refer to [2, 20] for more references.

Many of the studies mentioned above also apply in the case of a compact manifold without boundary or Neumann boundary conditions, which is the primary focus of this paper. However, in this case the principal eigenvalue is simply zero and corresponds to the constant eigenfunction. Instead one is interested in the speed of convergence of the solution to its average, the relaxation speed. A recent work of Franke [12] provides estimates on the heat kernels corresponding to the incompressible drift and diffusion on manifolds, but these estimates lead to upper bounds on $\|\varphi^A(1) - \overline{\varphi}\|$ which essentially do not improve as $A \to \infty$. One way to study the convergence speed is to estimate the spectral gap – the difference between the principal eigenvalue and the real part of the next eigenvalue. To the best of our knowledge, there is very little known about such estimates in the context of (1); see [18] p. 251 for a discussion. Neither probabilistic methods nor PDE methods of [2] seem to apply in this situation, in particular because the eigenfunction corresponding to the eigenvalue(s) with the second smallest real part is no longer positive and the eigenvalue itself does not need to be real. Moreover, even if the spectral gap estimate were available, generally it only yields a limited asymptotic in time dynamical information of type (2), and how fast the long time limit is achieved may depend on A. Part of our motivation for studying the advection-enhanced diffusion comes from the applications to quenching in reaction-diffusion equations (see e.g. [3, 9, 21, 25, 29]). For these applications, one needs estimates on the A-dependent L^∞ norm decay at a fixed positive time, the type of information the bound like (2) does not provide. We are aware of only one case where enhanced relaxation estimates of this kind are available. It is the recent work of Fannjiang, Nonnemacher and Wolowski [7, 8], where such estimates are provided in the discrete setting (see also [18] for some related earlier references). In these papers a unitary evolution step (a certain measure preserving map on the torus) alternates with a dissipation step, which, for example, acts simply by multiplying the Fourier coefficients by damping factors. The absence of sufficiently regular eigenfunctions appears as a key for the lack of enhanced relaxation in this particular class of dynamical systems. In [7, 8], the authors also provide finer estimates of the dissipation time for particular classes of toral automorphisms (that is, they estimate how many steps are needed to reduce the L^2 norm of the solution by a factor of two if the diffusion strength is ϵ).

Our main goal in this paper is to provide a review of recent work that addresses a question of sharp characterization of incompressible flows that are relaxation enhancing, in a quite general setup. The following natural definition has been introduced in [4] as a measure of the flow efficiency in improving the solution relaxation.

Definition 1. Let M be a smooth compact Riemannian manifold. The incompressible flow u on M is called relaxation enhancing if for every $\tau > 0$ and $\delta > 0$, there exist $A(\tau, \delta)$ such that for any $A > A(\tau, \delta)$ and any $\varphi_0 \in L^2(M)$ with $\|\varphi_0\|_{L^2(M)} = 1$ we have

$$\|\varphi^A(\cdot, \tau) - \overline{\varphi}\|_{L^2(M)} < \delta, \tag{3}$$

where $\varphi^A(x, t)$ is the solution of (1) and $\overline{\varphi}$ the average of φ_0.

Remarks.

1. In [4] it was shown that the choice of the L^2 norm in the definition is not essential and can be replaced by any L^p-norm with $1 \leq p \leq \infty$.
2. It follows from the proofs of our main results that the relaxation enhancing class is not changed even when we allow the flow strength that ensures (3) to depend on φ_0, that is, if we require (3) to hold for all $\varphi_0 \in L^2(M)$ with $\|\varphi_0\|_{L^2(M)} = 1$ and all $A > A(\tau, \delta, \varphi_0)$.

The main approach is to bypass the issue of the spectral gap, and work directly with dynamical estimates. The first result we describe has been proved in [4].

Theorem 2. *Let M be a smooth compact Riemannian manifold. A Lipschitz continuous incompressible flow $u \in \mathrm{LIP}(M)$ is relaxation enhancing if and only if the operator $u \cdot \nabla$ has no eigenfunctions in $H^1(M)$, other than the constant function.*

Any incompressible flow $u \in \mathrm{LIP}(M)$ generates a unitary evolution group U^t on $L^2(M)$, defined by $U^t f(x) f(\Phi_{-t}(x))$. Here $\Phi_t(x)$ is a measure preserving transformation associated with the flow, defined by $\frac{d}{dt}\Phi_t(x) = u(\Phi_t(x))$, $\Phi_0(x) = x$. Recall that a flow u is called weakly mixing if the corresponding operator U has only continuous spectrum. The weakly mixing flows are ergodic, but not necessarily mixing (see e.g. [5]). There exist fairly explicit examples of weakly mixing flows (see e.g. [1, 10, 11, 23, 26, 27]). A direct consequence of Theorem 2 is the following corollary.

Corollary 3. *Any weakly mixing incompressible flow $u \in \mathrm{LIP}(M)$ is relaxation enhancing.*

Theorem 2 in its turn follows from quite general abstract criterion, which we are now going to describe. Let Γ be a self-adjoint, positive, unbounded operator with a discrete spectrum on a separable Hilbert space H. Let $0 < \lambda_1 \leq \lambda_2 \leq \cdots$ be the eigenvalues of Γ, and e_j the corresponding orthonormal eigenvectors forming a basis in H. The (homogeneous) Sobolev space $H^m(\Gamma)$ associated with Γ is formed by all vectors $\psi = \sum_j c_j e_j$ such that

$$\|\psi\|^2_{H^m(\Gamma)} \equiv \sum_j \lambda_j^m |c_j|^2 < \infty.$$

Note that $H^2(\Gamma)$ is the domain $D(\Gamma)$ of Γ. Let L be a self-adjoint operator such that, for any $\psi \in H^1(\Gamma)$ and $t > 0$ we have

$$\|L\psi\|_H \leq C\|\psi\|_{H^1(\Gamma)} \quad \text{and} \quad \|e^{iLt}\psi\|_{H^1(\Gamma)} \leq B(t)\|\psi\|_{H^1(\Gamma)} \tag{4}$$

with both the constant C and the function $B(t) < \infty$ independent of ψ and $B(t) \in L^2_{\text{loc}}(0, \infty)$. Here e^{iLt} is the unitary evolution group generated by the self-adjoint operator L.

Consider a solution $\varphi^A(t)$ of the Bochner differential equation

$$\frac{d}{dt}\varphi^A(t) = iAL\varphi^A(t) - \Gamma\varphi^A(t), \quad \varphi^A(0) = \varphi_0. \tag{5}$$

Similarly to the Definition 1 above, we say

Definition 4. We call evolution corresponding to (5) relaxation enhancing if for any $\tau, \delta > 0$ there exists $A(\tau, \delta)$ such that for any $A > A(\tau, \delta)$ and any $\varphi_0 \in H$ with $\|\varphi_0\|_H = 1$, the solution $\varphi^A(t)$ of the equation (5) satisfies $\|\varphi^A(\tau)\|_H < \delta$.

Theorem 5. *Let Γ be a self-adjoint, positive, unbounded operator with a discrete spectrum and let a self-adjoint operator L satisfy conditions* (4)*. Then the following two statements are equivalent*:

- *The evolution is relaxation enhancing*
- *The operator L has no eigenvectors lying in $H^1(\Gamma)$.*

Remark. Here L corresponds to $iu \cdot \nabla$ (or, to be precise, a self-adjoint operator generating the unitary evolution group U^t which is equal to $iu \cdot \nabla$ on $H^1(M)$), and Γ to $-\Delta$ in Theorem 2, with $H \subset L^2(M)$ the subspace of mean zero functions.

Theorem 5 provides a sharp answer to the general question of when a combination of fast unitary evolution and dissipation produces a significantly stronger dissipative effect than dissipation alone. It can be useful in any model describing a physical situation which involves fast unitary dynamics with dissipation (or, equivalently, unitary dynamics with weak dissipation). The proof uses ideas from quantum dynamics, in particularly the RAGE theorem (see e.g., [6]) describing evolution of a quantum state belonging to the continuous spectral subspace of a self-adjoint operator.

A natural concern is if the existence of rough eigenvectors of L is consistent with the condition (4) which says that the dynamics corresponding to L preserves $H^1(\Gamma)$. In [4], this question was answered in the affirmative by providing examples where rough eigenfunctions exist yet (4) holds. One of the examples involved a discrete version of the celebrated Wigner-von Neumann construction of an imbedded eigenvalue of a Schrödinger operator [28]. Moreover, another example constructed in [4] involved a smooth flow on the two dimensional torus $\mathbb{T}^2$ with discrete spectrum and rough (not $H^1(\mathbb{T}^2)$) eigenfunctions—the idea of this example essentially goes back to Kolmogorov [23]. Thus, the issue of rough eigenfunctions is not moot and result of Theorem 5 is precise.

The third result we are going to describe is a natural extension of Theorem 5 and Theorem 2 to the case of time periodic flows [22]. Clearly, most flows in practice are time dependent, and it is important to understand this more general case. The time periodic situation is a natural first step. Without loss of generality, we will assume

that the period in time is equal to one, and will state only the general result. Let $L(t)$ be a self-adjoint (for any t) operator, periodic with respect to t with period 1 and such that the following two conditions hold.

Condition 1. For any $\psi \in H^1(\Gamma)$ we have

$$\|L(t)\psi\| \leq C_0\|\psi\|_1 \tag{6}$$

with constant C_0 independent of t.

Denote by $U(t, s)$ unitary group associated with equation

$$\frac{d}{dt}\psi(t) = iL(t)\psi(t). \tag{7}$$

Thus, $U(t, s)\psi(s) = \psi(t)$. Due to periodicity of $L(t)$ we have $U(t + 1, s + 1) = U(t, s)$. For period operator $U(1, 0)$ we use the notation V.

Condition 2. For any $\psi \in H^1(\Gamma)$ we have

$$\|U(s + t, s)\psi\|_1 \leq B(t, s)\|\psi\|_1 \tag{8}$$

with constant $B(t, s) < \infty$ (periodic in s) such that for any $X > 0$

$$\sup_{t\in[0,X]} \sup_{s\in[0,1]} B(t, s) \leq C_*(X) < \infty. \tag{9}$$

Consider the equation

$$\frac{d}{dt}\varphi^A(t) = iL(t)\varphi^A(t) - \Gamma\varphi^A(t), \quad \varphi^A(0) = \varphi_0, \tag{10}$$

where Γ is as before. Then the main result is the following [22]:

Theorem 6. *Under Conditions 1 and 2 evolution is relaxation enhancing* (*in the sense of Definition 4*) *if and only if the unitary operator V has no eigenfunctions in $H^1(\Gamma)$.*

Thus the relaxation enhancement for time periodic flows is equivalent to the investigation of the eigenfunctions of the time one map V. It is interesting to note that in the case of a fluid flow $u(x, t)$, the problem reduces to studying a different flow of special form in one extra space dimension. Namely, let us denote the unit circle by $\mathbb{T}$. In the Hilbert space $\mathcal{H} := L_2(\mathbb{T}, H)$—functions on $\mathbb{T}$ which are L_2 with values in H consider unitary evolution $e^{iK\sigma}$ defined by

$$e^{iK\sigma} f(t) := U(t, t - \sigma) f(t - \sigma). \tag{11}$$

We denote by K the self-adjoint generator of the unitary group $e^{iK\sigma}$. Formally,

$$K := i\frac{d}{dt} + L(t). \tag{12}$$

Then one can prove [22].

Theorem 7. *Operator V has an eigenfunction in $H^1(\Gamma)$ if and only if operator K has an eigenfunction $f(x,t)$ in $\mathcal{H}^1 := L_2(\mathbb{T}, H^1(\Gamma)) \cap H^1(\mathbb{T}, H)$.*

Finally, the last result we are going to mention deals with relaxation enhancement in non-compact regions (specifically, $\mathbb{R}^2$ and $\mathbb{R} \times \mathbb{T}$). Given an incompressible Lipshitz flow v in a domain D, let us denote $P_t(v)$ the solution operator for the equation

$$\psi_t + v \cdot \nabla \psi = \Delta \psi, \quad \psi(0) = \psi_0 \tag{13}$$

on D. That is, $P_t(v)\psi_0 = \psi(\cdot, t)$ when ψ solves (13). The following theorem has been proved in [30]:

Theorem 8. *Let u be a periodic, incompressible, Lipshitz flow on $D = \mathbb{R}^2$ or $D = \mathbb{R} \times \mathbb{T}$ with a cell of periodicity C, and let φ^A solve (1) in D. The following are equivalent.*

(i) *For some $1 \le p \le q \le \infty$ and each $\tau > 0$, $\varphi_0 \in L^p(D)$,*

$$\|\varphi^A(\cdot, \tau)\|_{L^p(D)} \to 0 \quad \text{as } A \to \infty. \tag{14}$$

(ii) *For any $1 \le p \le q \le \infty$ such that $p < \infty$ and $q > 1$, and each $\tau > 0$, $\varphi_0 \in L^p(D)$,*

$$\|\varphi^A(\cdot, \tau)\|_{L^p(D)} \to 0 \quad \text{as } A \to \infty.$$

(iii) *For any $1 \le p \le q \le \infty$ and each $\tau > 0$,*

$$\|P_\tau(Au)\|_{L^p(D) \to L^q(D)} \to 0 \quad \text{as } A \to \infty.$$

(iv) *No bounded open subset of D is invariant under u and any eigenfunction of u on C that belongs to $H^1(C)$ is a first integral of u.*

The first three statements in the above theorem provide essentially different equivalent definitions of relaxation enhancement (which may be more reasonable to call dissipation enhancement in this setting, since the limiting value is going to be equal to zero). The fourth is a sharp characterization of flows that provide such dissipation enhancement on D. An interesting aspect of this theorem is that in the non-compact setting the class of relaxation enhancing flows includes some flows with first integrals on the cell, such as shear flows in the infinite direction which have a plateau. The paper [30] contains some other interesting examples and generalizations.

In the following section we sketch some of the main ideas behind the proof of the Theorems 2, 5, 6 and 8.

2 The Heart of the Matter

While we are not going to present detailed proofs, we would like to outline, or perhaps even just illustrate, the main idea behind the general criterion Theorem 5

and its connection with estimates on wavepacket spreading in quantum mechanics. For this purpose, it is convenient to switch to an equivalent formulation with small parameter $\epsilon = A^{-1}$. Namely, we will look at the equation

$$\varphi_t^\epsilon = iL\varphi^\epsilon - \epsilon\Gamma\varphi^\epsilon, \quad \varphi^\epsilon(0) = \varphi_0. \tag{15}$$

The question then becomes under what conditions on L for any $\tau, \delta > 0$ we can find sufficiently small $\epsilon(\tau, \delta)$ such that for any $\epsilon < \epsilon(\tau, \delta)$ we have $\|\varphi^\epsilon(\tau/\epsilon)\| < \delta$?

One direction of the Theorem 5 is rather straightforward. If there exists $\varphi \in H^1$ such that $L\varphi = \lambda\varphi$, then it is not difficult to show that L cannot be relaxation enhancing. It suffices to take the initial data φ_0 equal to φ and carry out a few elementary estimates on the equation [4].

The converse direction is trickier. The evolution due to L is unitary, while unperturbed dissipative part due to $\epsilon\Gamma$ delivers decay by just a fixed factor on the time scale of the order ϵ^{-1}—if there is no mixing by L. Thus enhanced dissipation can only happen if the unitary evolution transports the initial data to progressively higher harmonics of Γ. Since at any time t we have

$$\partial_t \|\varphi^\epsilon\|^2 = \epsilon\|\varphi^\epsilon(s)\|_1^2, \tag{16}$$

we just need to obtain sufficiently strong lower bound (perhaps on average) for the H^1 norm of the solution. Let us recall the following statement, well known in mathematical quantum mechanics as the RAGE theorem (in honor of Ruelle, Ahmrein, Georgescu and Enss [6]).

Theorem 9. *Assume L is a self-adjoint operator, and denote P_c the projector on the continuous spectral subspace. Let C be a compact operator. Then for any $\varphi \in H$, we have*

$$\frac{1}{T}\int_0^T \|C\exp(iLt)P_c\varphi\|^2\,dt \to 0 \tag{17}$$

as $T \to \infty$.

This is a precise formulation of a well known informal principle saying that the quantum evolution corresponding to continuous spectrum is unbounded. Indeed, think of a discrete case, where $H = l^2(Z^d)$, and take K equal to a projection on a ball of radius R. Then the statement of the Theorem says that the wavepacket, on average, will stay out of this ball for large times. The proof is based on a well known and simple Wiener theorem saying that if μ is a probability measure with point masses at a_i and $\hat{\mu}$ is its Fourier transform, then

$$\frac{1}{T}\int_0^T |\hat{\mu}(t)|^2\,dt \to \sum_i \mu(a_i)^2$$

as $T \to \infty$. Clearly, the unboundedness of the unitary dynamics should be very relevant in our case, where the natural basis is given by the eigenfunctions of Γ and the goal is to show that the evolution migrates to high modes and dissipates.

Let us now consider the case where our operator L has purely continuous spectrum. In this case, the proof is especially transparent. The key are the following two lemmas. The first lemma ensures that the solution of (15) stays close for a while to the unitary evolution $\varphi^0(t) = \exp(iLt)\varphi_0$.

Lemma 10. *Assume the conditions* (4) *hold. Let* $\varphi^0(t), \varphi^\epsilon(t)$ *be solutions of*

$$(\varphi^0)'(t) = iL\varphi^0(t), \quad (\varphi^\epsilon)'(t) = (iL - \epsilon\Gamma)\varphi^\epsilon(t),$$

satisfying $\varphi^0(0) = \varphi^\epsilon(0) = \varphi_0 \in H^1$. *Then we have*

$$\frac{d}{dt}\|\varphi^\epsilon(t) - \varphi^0(t)\|^2 \le \frac{1}{2}\epsilon\|\varphi^0(t)\|_1^2 \le \frac{1}{2}\epsilon B^2(t)\|\varphi_0\|_1^2. \tag{18}$$

As a consequence,

$$\|\varphi^\epsilon(t) - \varphi^0(t)\|^2 \le \frac{1}{2}\epsilon\|\varphi_0\|_1^2 \int_0^\tau B^2(t)\,dt$$

for any time $t \le \tau$.

This lemma can be proved by elementary arguments [4].

The second lemma is an upgraded version of the RAGE theorem. Recall that we denote by $0 < \lambda_1 \le \lambda_2 \le \cdots$ the eigenvalues of the operator Γ and by $e_1, e_2, \ldots$ the corresponding orthonormal eigenvectors. Let us also denote by P_N the orthogonal projection on the subspace spanned by the first N eigenvectors $e_1, \ldots, e_N$ and by $S = \{\varphi \in H : \|\varphi\| = 1\}$ the unit sphere in H. The following lemma shows that if the initial data lies in the continuous spectrum of L then the L-evolution will spend most of time in the higher modes of Γ.

Lemma 11. *Let* $K \subset S$ *be a compact set. For any* $N, \sigma > 0$, *there exists* $T_c(N, \sigma, K)$ *such that for all* $T \ge T_c(N, \sigma, K)$ *and any* $\varphi \in K$, *we have*

$$\frac{1}{T}\int_0^T \|P_N e^{iLt} P_c\varphi\|^2\,dt \le \sigma\|\varphi\|^2. \tag{19}$$

An important aspect of this lemma is the uniformity of the estimate in $\varphi \in K$.

Given these two lemmas, here is a sketch of the proof of Theorem 5.

Fix $\delta, \tau > 0$. Take $\sigma = 1/10$, and choose N so that

$$\exp(-\lambda_N\tau/10) < \delta. \tag{20}$$

We will also assume that λ_N is chosen to be larger than one. Define a compact set

$$K = \left\{\varphi \in H \middle| \|\varphi\|_1^2 \leq \lambda_N \|\varphi\|^2\right\}.$$

Define $\tau_1 = T_c(N, 1/10, K)$. Finally, take any $\epsilon < \epsilon(\tau, \delta)$ where the latter is defined by a condition

$$\epsilon(\tau, \delta) \int_0^{\tau_1} B^2(t)\, dt \leq \frac{1}{20\lambda_N}. \tag{21}$$

Assume that we have $\|\varphi^\epsilon(t)\|_1^2 > \lambda_N \|\varphi^\epsilon(t)\|^2$ for any t in some interval $[a, b] \subset [0, \tau/\epsilon]$. Then from (16), it follows that

$$\|\varphi^\epsilon(b)\|^2 \leq \exp(-\epsilon\lambda_N(b-a))\|\varphi^\epsilon(a)\|^2. \tag{22}$$

In particular, if we could take $[a, b] = [0, \tau/\epsilon]$, then by (20) the norm of the solution will be less than δ at $t = \tau/\epsilon$.

Now let us examine what happens if at any time τ_0 we have $\|\varphi^\epsilon(\tau_0)\|_1^2 \leq \lambda_N \|\varphi^\epsilon(\tau_0)\|^2$. For the sake of transparency, henceforth we will denote $\varphi^\epsilon(\tau_0) = \varphi_0$. On the interval $[\tau_0, \tau_0 + \tau_1]$, consider the function $\varphi^0(t)$ satisfying $\frac{d}{dt}\varphi^0(t) = iL\varphi^0(t)$, $\varphi^0(\tau_0) = \varphi_0$. Note that by the choice of ϵ, τ_0, (21), and Lemma 18, we have

$$\|\varphi^\epsilon(t) - \varphi^0(t)\|^2 \leq \frac{1}{10}\|\varphi_0\|^2 \tag{23}$$

for all $t \in [\tau_0, \tau_0 + \tau_1]$. Our choice of τ_1 implies that

$$\frac{1}{\tau_1} \int_{\tau_0}^{\tau_0+\tau_1} \|P_N\varphi^0(t)\|^2\, dt \leq \frac{1}{10}\|\varphi_0\|^2. \tag{24}$$

Taking into account that the evolution $\varphi^0(t)$ is unitary, it follows that

$$\frac{1}{\tau_1} \int_{\tau_0}^{\tau_0+\tau_1} \|(I - P_N)\varphi^0(t)\|^2\, dt \geq \frac{9}{10}\|\varphi_0\|^2. \tag{25}$$

Using (23), we conclude that

$$\frac{1}{\tau_1} \int_{\tau_0}^{\tau_0+\tau_1} \|(I - P_N)\varphi^\epsilon(t)\|^2\, dt \geq \frac{1}{2}\|\varphi_0\|^2. \tag{26}$$

This estimate implies that

$$\int_{\tau_0}^{\tau_0+\tau_1} \|\varphi^\epsilon(t)\|_1^2\, dt \geq \frac{\lambda_N\tau_1}{2}\|\varphi_0\|^2. \tag{27}$$

Combining (27) with (16) yields

$$\|\varphi^{\epsilon}(\tau_0+\tau_1)\|^2 \leq \left(1-\frac{\lambda_N \epsilon \tau_1}{2}\right)\|\varphi^{\epsilon}(\tau_0)\|^2 \leq e^{-\lambda_N \epsilon \tau_1/2}\|\varphi^{\epsilon}(\tau_0)\|^2. \tag{28}$$

The whole interval $[0, \tau/\epsilon]$ can now be split into a union of intervals such that either (22) or (28) applies. Thus we obtain (assuming $\|\varphi_0\| = 1$)

$$\|\varphi^{\epsilon}(\tau/\epsilon)\|^2 \leq \exp(-\lambda_N \tau/2) < \delta^2,$$

finishing the proof in this case.

Including the point spectrum case is technically tricky, and we refer to [4] for the complete treatment. However, the argument that we just provided illustrates some key ideas well. The overall plan of the argument is flexible enough to also apply in the time periodic case [22].

3 Open Questions

In this section, we briefly discuss some open questions. There are many natural directions in which one can pursue further developments. For example, discrete time version, more precise quantitative estimates of the enhancement and links to relevant properties of the dynamical systems and nonlinear dissipation are all of interest. However here we will focus on describing in detail just two questions—which are most likely hardest but are also in our opinion very interesting.

1. The spectral analog. The first question is to obtain estimates on the spectral gap in this truly non-selfadjoint situation. The issue is really twofold. Consider the operator

$$H_A = iAL - \Gamma.$$

Let us denote λ_1^A the eigenvalue with the minimal real part (one of those eigenvalues if it is not unique). Obtaining any analytical estimate on the $\Re\lambda_1^A$ of the operator H_A would require completely new ideas. As we mentioned in the introduction, the current estimates available in the Dirichlet boundary condition setting for the flow operator depend critically on the fact that the principal eigenvalue is real and the corresponding eigenfunction is positive. Clearly, such properties have no analog in general for (3). The second question is if the link between dynamical behavior and spectral gap remains true in this case. A natural conjecture is that $\limsup_{A\to\infty} \Re\lambda_1^A < \infty$ if and only if L has $H^1(\Gamma)$ eigenfunctions and if and only if evolution is not relaxation enhancing. In fact, the "only if" direction can be proved similarly to [2]; it is the "if" direction that looks difficult. Finding what the above limit (if it exists and finite) is going to be equal to is another interesting problem.

Generally, it is well known that in non-selfadjoint spectral analysis, "anything can happen". The question is if the natural problem that we are looking at has sufficient structure to still possess some nice properties.

2. Examples of time-dependent flows. Theorem 6 provides a simple characterization of the time-periodic relaxation enhancing flows. Intuitively, it is clear that time dependence of the flow is likely to improve its mixing properties in many situations. A very reasonable question is therefore the following:

Find an example of a 2D incompressible flow $u(x, y, t)$, *periodic both in space and time with period* 1, *such that for each fixed* t_0, $u(x, y, t_0)$ *is not relaxation enhancing* (*for instance, the mean of u is zero*) *but the time dependent flow* $u(x, y, t)$ *is relaxation enhancing.*

We were unable to find such examples in the existing literature. One approach suggested by Theorem 6, would be to start from a relaxation enhancing (for example, mixing) time one map, and try to build a flow leading to it. However, most explicit mixing maps on the torus that appear in the literature, such as simple Anosov diffeomorphisms, are not homotopic to the identity map—and so cannot be realized by a smooth flow on the torus. We believe that the above question is interesting purely from the dynamical systems point of view, independently of its applications to the advection-diffusion. Note added in proof: after this review was submitted, an example answering this question has been constructed in [22].

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Random Schrödinger Operators: Localization and Delocalization, and All That

François Germinet and Abel Klein

Abstract In this review we consider random Schrödinger operators which are ergodic and have the property of independence at a distance. The basic examples are the Anderson tight-binding model, the continuum Anderson Hamiltonian, the random Landau Hamiltonian, and the Poisson Hamiltonian. We review localization and delocalization for these random Schrödinger operators, discussing the metal-insulator transition and its mathematical interpretations: the spectral metal-insulator transition and the dynamical metal-insulator transition. The occurrence of the dynamical metal-insulator transition in the random Landau Hamiltonian is reviewed.

1 Random Schrödinger Operators

Consider an electron moving in a medium with random impurities. For a fixed configuration of the impurities, labeled by a point ω in a probability space $(\Omega, \mathbb{P})$, this motion is described by the Schrödinger equation

$$-i\,\partial_t\,\psi_t\,H_\omega\,\psi_t \tag{1}$$

on the Hilbert space $\mathscr{H} = \mathrm{L}^2(\mathbb{R}^d)$, where the Hamiltonian is a random Schrödinger operator:

$$H_\omega := H_0 + V_\omega, \tag{2}$$

with $H_0 = -\Delta$, the d-dimensional Laplacian operator and V_ω a random potential. (The free Hamiltonian H_0 may be modified to include a magnetic field or a back-

François Germinet
Département de Mathématiques, Univ. Cergy-Pontoise, CNRS UMR 8088, IUF, 95000 Cergy-Pontoise, France, e-mail: germinet@math.u-cergy.fr

Abel Klein
Department of Mathematics, University of California, Irvine, CA 92697-3875, USA, e-mail: aklein@uci.edu

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ground periodic potential, or both.) This quantum mechanical system is also studied in the tight-binding approximation, where the Hilbert space is $\mathscr{H} = \ell^2(\mathbb{Z}^d)$ and Δ is the discrete Laplacian.

Mathematical considerations require H_ω to be a random self-adjoint operator: H_ω is a self-adjoint operator for $\mathbb{P}$-a.e. ω (usually bounded from below), and the mappings $\omega \to f(H_\omega)$ are weakly (and hence strongly) measurable for all bounded Borel measurable functions f on $\mathbb{R}$.

Physical considerations require the random Schrödinger operator H_ω to be homogeneous and ergodic with respect to translations by elements of $\mathbb{Z}^d$ (or $\mathbb{R}^d$): there exists an ergodic family $\{\tau_y;\ y \in \mathbb{Z}^d\}$ of measure preserving transformations on $(\Omega, \mathbb{P})$ such that

$$U(y) H_\omega U(y)^* = H_{\tau_y(\omega)} \quad \text{for all } y \in \mathbb{Z}^d, \tag{3}$$

where $(U(y)\varphi)(x) = \varphi(x-y)$. (If there is a magnetic field, translations are replaced by magnetic translations.)

In this review a random Schrödinger operator H_ω will always be an ergodic random self-adjoint operator. An important property is the existence of a nonrandom set Σ such that $\sigma(H_\omega) = \Sigma$ for $\mathbb{P}$-a.e. ω, where $\sigma(A)$ denotes the spectrum of the operator A. In addition, the decomposition of $\sigma(H_\omega)$ into pure point spectrum $\sigma_{pp}(H_\omega)$, absolutely continuous spectrum $\sigma_{ac}(H_\omega)$, and singular continuous spectrum $\sigma_{sc}(H_\omega)$ is also independent of the choice of ω with probability one, i.e., there are nonrandom sets Σ_{pp}, Σ_{ac} and Σ_{sc}, such that $\sigma_{pp}(H_\omega) = \Sigma_{pp}$, $\sigma_{ac}(H_\omega) = \Sigma_{ac}$, and $\sigma_{sc}(H_\omega) = \Sigma_{sc}$ with probability one. (See [85, 77, 60, 86, 16, 25].)

In many physical systems the random impurities located in disjoint (and sufficiently apart) regions are stochastically independent. This will be assumed in this review. As a consequence, the corresponding random Schrödinger operators possess the property of independence at a distance: events based on disjoint (and sufficiently apart) regions will be independent.

In this review we consider localization and delocalization for these random Schrödinger operators. We introduce the basic examples, and review localization and delocalization, discussing the metal-insulator transition and its mathematical interpretations: the spectral metal-insulator transition and the dynamical metal-insulator transition. The occurrence of the dynamical metal-insulator transition in the random Landau Hamiltonian is reviewed. We do not discuss the proofs, but references are provided. The references will also include results of similar type with somewhat different hypotheses.

2 Basic Examples of Random Schrödinger Operators

We consider H_ω as in (2) on a Hilbert space $\mathscr{H}$, where $\mathscr{H}$ will be either $\mathrm{L}^2(\mathbb{R}^d)$ or $\ell^2(\mathbb{Z}^d)$. We fix the following notation:

- $\omega = \{\omega_j\}_{j\in\mathbb{Z}^d}$ are independent identically distributed random variables with a common probability distribution μ whose support is compact with at least two points.
- $u(x)$ is a nonnegative bounded measurable function on $\mathbb{R}^d$ with compact support, with $u(x) \geq \delta > 0$ in a ball centered at $x = 0$.

The assumption that the probability distribution μ has compact support may be often replaced by less restrictive conditions, but we will assume it to simplify the exposition. In addition, most of the mathematical results require a regularity assumption: the common probability distribution μ has a bounded density ρ. If μ satisfies this assumption, the corresponding random Schrödinger operator will be called *regular*.

We will now introduce the random Schrödinger operators we discuss in this review.

2.1 The Anderson (Tight-Binding) Model

This is the original random Schrödinger operator introduced in [10]. It acts on the lattice, i.e., $\mathscr{H} = \ell^2(\mathbb{Z}^d)$. $H_0 = -\Delta$, with Δ the centered discrete Laplacian:

$$(\Delta\varphi)(x) := -\sum_{y\in\mathbb{Z}^d;\, |x-y|=1} \varphi(y) \quad \text{for } \varphi \in \ell^2(\mathbb{Z}^d); \tag{4}$$

note $\sigma(-\Delta) = [-2d, 2d]$. The random potential is simply

$$V_\omega(j) = \omega_j \quad \text{for all } j \in \mathbb{Z}^d. \tag{5}$$

2.2 The (Continuum) Anderson Hamiltonian

This is the continuum version of the Anderson model; it describes the motion of an electron in a disordered crystal (a random alloy). Here $\mathscr{H} = \mathrm{L}^2(\mathbb{R}^d)$, $H_0 = -\Delta + V_{\mathrm{per}}$, where V_{per} is a bounded periodic potential with period $q \in \mathbb{N}$, and the random potential is

$$V_\omega(x) = \sum_{j\in\mathbb{Z}^d} \omega_j\, u(x - j) \quad \text{for all } x \in \mathbb{R}^d. \tag{6}$$

2.3 The Random Landau Hamiltonian

Here $\mathscr{H} = \mathrm{L}^2(\mathbb{R}^2)$ and we have a magnetic field. The free Hamiltonian is

$$H_0 = H_B := (-i\nabla - \mathbf{A})^2, \tag{7}$$

where $B > 0$ is the strength of the magnetic field, $\mathbf{A} = \frac{B}{2}(x_2, -x_1)$ is the vector potential, and V_ω is the random potential in (6). The covariance relation (3) holds with respect to magnetic translations, defined by

$$(U(y)\varphi)(x) = \mathrm{e}^{-i\frac{B}{2}(x_2y_1 - x_1y_2)}\varphi(x - y). \tag{8}$$

The random Landau Hamiltonian is $\mathbb{Z}^2$-ergodic with respect to these magnetic translations. It appears in the study of the quantum Hall effect (cf. [58, 95, 13, 14]).

2.4 The Poisson Hamiltonian

Here $\mathscr{H} = \mathrm{L}^2(\mathbb{R}^2)$, $H_0 = -\Delta$, and the random potential is

$$V_{\mathbf{X}}(x) = \sum_{j \in \mathbf{X}} u(x - j), \tag{9}$$

where $\mathbf{X}$ is a (homogeneous) Poisson process on $\mathbb{R}^d$. The Poisson Hamiltonian is $\mathbb{R}^d$-ergodic; it describes the motion of an electron in a disordered amorphous material (cf. [81]).

3 The Metal-Insulator Transition

The following picture is widely accepted in the Physics literature [10, 3, 82]:

- In dimension $d \geq 3$, a random Schrödinger operator exhibits a transition from an *insulator region*, characterized by *localized states*, to a very different *metallic region*, characterized by *extended states*. The energy at which this *metal-insulator transition* occurs is called the *mobility edge* (E_{me}).

  $\Sigma = \sigma(H_\omega)$:

  insulator | metal

  E_{me}

- If $d = 1$ there is no transition, there are only localized states.
- If $d = 2$ it is also believed that there are only localized states.

4 The Spectral Metal-Insulator Transition

The usual mathematical interpretation of the metal-insulator transition is a spectral transition using the following dictionary:

- The *insulator region* is the spectral region where the random Schrödinger operator exhibits *Anderson localization*, that is, *pure point spectrum with exponentially decaying eigenstates*.
- The *metallic region* is the spectral region where the random Schrödinger operator has *absolutely continuous spectrum*.

4.1 Anderson Localization

The random Schrödinger operator H_ω is said to exhibit *Anderson localization* in an interval I, where $I^\circ \cap \Sigma \neq 0$, if there exists $m > 0$ such that the following holds with probability one:

- H_ω has pure point spectrum in I.
- If φ is an eigenfunction of H_ω with eigenvalue $E \in I$, then φ is exponentially localized with rate of decay m, more precisely,

$$\|\chi_x \varphi\| \leq C_{\omega,\varphi}\, \mathrm{e}^{-m|x|} \quad \text{for all } x \in \mathbb{Z}^d. \tag{10}$$

A note about notation: I° is the interior of I. χ_B denotes the characteristic function of the set B. χ_x denotes the characteristic function of the cube of side 1 centered at x, that is, the characteristic function of the set $x+[-\frac{1}{2}, \frac{1}{2}]^d$. Note that in the lattice we have $\chi_x = \chi_{\{x\}}$, so $\|\chi_x \varphi\| = |\varphi(x)|$.

Let I be the interval of Anderson localization. If $I = \mathbb{R}$ we will say 'for all energies'. If $I = [E_{\inf}, E_1]$ with $E_{\inf} := \inf \Sigma < E_1$ we will say 'at the bottom of the spectrum. (Note that we always have $E_{\inf} > -\infty$ under our hypotheses.) For the Anderson model, Σ is a compact set under our hypotheses, so we can also talk about 'the top of the spectrum'; we will use 'at the edges of the spectrum' to mean at the bottom and at the top of the spectrum.

We also introduce a disorder parameter $\lambda > 0$, and set $H_{\omega,\lambda} = H_0 + \lambda V_\omega$. By Anderson localization at high disorder for H_ω we will mean Anderson localization for $H_{\omega,\lambda}$ for all sufficiently large λ.

Anderson localization was first proven for a particular one-dimensional continuum random Schrödinger operator [55]. The random potential is given by a Morse function of Brownian motion in a compact manifold. Anderson localization was proven for all energies, i.e., on $\mathbb{R}$.

We will review the results on Anderson localization for the Anderson model, the Anderson Hamiltonian, and the Poisson Hamiltonian. We will also discuss the multiplicity of the eigenvalues in intervals of Anderson localization. The random Landau Hamiltonian will be discussed in Sect. 6.

4.1.1 Anderson Localization in the One-Dimensional Case

For $d = 1$ the widely accepted picture, Anderson localization at all energies, has been verified in great generality. It has been proven in the following cases:

- For a one-dimensional continuum random Schrödinger operator where the random potential is given by a Morse function of Brownian motion in a compact manifold; the first proof of Anderson localization [55].
- For the Anderson model:
  - For the regular model, i.e., μ with a bounded density [77, 72, 25].
  - For μ arbitrary [17, 87].
- For the Anderson Hamiltonian [27].
- For the Poisson Hamiltonian [93].

4.1.2 Anderson Localization in the Multi-Dimensional Case

For $d \geq 2$ Anderson localization has been proved as expected for $d \geq 3$; there are no results specific to $d = 2$. In more detail, for $d \geq 2$ we have:

- For the Anderson model, we have Anderson localization at the edges of the spectrum, and also at all energies for high disorder, as follows:
  - For μ with a bounded density, the regular Anderson model [38, 39, 32, 89, 96, 97, 90, 98, 5, 65, 35, 4, 6, 100, 75].
  - For μ Hölder continuous [17].
  - There are no results at this time for more singular μ.
- For the Anderson Hamiltonian, we always have localization at the bottom of the spectrum, or at a fixed interval at the bottom of the spectrum for high disorder. These results have been proven as follows:
  - For μ with a bounded density, the regular Anderson Hamiltonian [59, 20, 73, 36, 62, 63, 41, 44, 42, 7, 70].
  - For μ Hölder continuous [91, 92, 23].
  - For μ a Bernoulli distribution, the Bernoulli-Anderson model [15].
  - For μ arbitrary (nontrivial, with compact support) [47]. (For just spectral localization, i.e., pure point spectrum, see [9].)
- For the Poisson Hamiltonian, we have localization at the bottom of the spectrum, or at a fixed interval at the bottom of the spectrum for high disorder [49, 51, 50].

4.1.3 Multiplicity of Eigenvalues in Intervals of Anderson Localization

There is a general belief that eigenvalues in intervals of Anderson localization should be simple. The following is known:

- In $d = 1$ the multiplicity of an eigenvalue of a Schrödinger operator is at most two.

- The eigenvalues of a regular Anderson model in an interval of Anderson localization are simple [88, 71].
- The eigenvalues of an Anderson Hamiltonian in an interval of Anderson localization have finite multiplicity:
  - For μ with a bounded density, the regular Anderson Hamiltonian [20, 46].
  - For μ Hölder continuous [46].
  - For μ arbitrary (e.g., μ a Bernoulli distribution) [47].
- The eigenvalues of a Poisson Hamiltonian in an interval of Anderson localization have finite multiplicity [47].
- The eigenvalues of a regular Anderson Hamiltonian in an interval of Anderson localization at the bottom of the spectrum are simple [24].

4.2 Absolutely Continuous Spectrum

At this time there are no proofs of existence of absolutely continuous spectrum (or even continuous spectrum) for the random Schrödinger operators discussed in this review. The only results are for the special case of the Anderson model on the Bethe lattice (or Cayley tree: an infinite connected graph with no closed loops and a fixed degree at each vertex), where for small disorder the random operator has purely absolutely continuous spectrum in a nontrivial interval [66, 69, 68] (see also [8, 37]) and exhibits ballistic behavior [67]. These results hold for any probability distribution μ with a finite second moment.

4.3 The Spectral Metal-Insulator Transition for the Anderson Model on the Bethe Lattice

The Physics literature predicts a metal-insulator transition for the Anderson model on the Bethe lattice [2, 1, 78, 83, 84]. We have the following mathematical results the Anderson model on the Bethe lattice:

- For a probability distribution μ with a finite second moment and a bounded density, Anderson localization is proven at high disorder [5] and for large energies [4].
- For a probability distribution μ with a finite second moment, purely absolutely continuous spectrum is proven in a nontrivial interval for small disorder [66].

We thus obtain the existence of a spectral metal-insulator transition for a probability distribution μ with a finite second moment, a bounded density, and unbounded support, say $\operatorname{supp} \mu = \mathbb{R}$. In particular, there is a spectral metal-insulator transition if μ has a Gaussian distribution.

5 The Dynamical Metal-Insulator Transition

An alternative mathematical interpretation of the metal-insulator transition as a dynamical transition was introduced in [45, 43] using the following dictionary:

- The *insulator region* is the spectral region where the random Schrödinger operator exhibits *dynamical localization*.
- The *metallic region* is the spectral region where the random Schrödinger operator exhibits *dynamical delocalization*.

5.1 Dynamical Localization

The intuitive physical notion of localization has also a dynamical interpretation: a wave packet, initially localized in space and in energy, should remain localized under time evolution. In a periodic medium there is ballistic motion: the n-th moment of an initially localized wave packet grows with time as t^n (cf. [11, 64]). In a random medium the insulator regime should exhibit *dynamical localization*: all moments of a wave packet, initially localized both in space and in energy (in the insulator region), remain uniformly bounded under time evolution.

Anderson and dynamical localization are not equivalent notions. Dynamical localization implies pure point spectrum by the RAGE Theorem (cf. the argument in [25, Theorem 9.21]), but the converse is not true. Dynamical localization is actually a strictly stronger notion than spectral localization (pure point spectrum): Anderson localization can take place whereas a quasi-ballistic motion is observed [30, 31].

If $x \in \mathbb{R}^d$ we write $\langle x\rangle = \sqrt{1+|x|^2}$. We use $\langle X\rangle$ to denote the operator given by multiplication by the function $\langle x\rangle$. By χ_x we denote the characteristic function of the cube of side 1 centered at $x \in \mathbb{R}^d$. Given an open interval $I \subset \mathbb{R}$, we denote by $C_c^\infty(I)$ the class of real valued infinitely differentiable functions on $\mathbb{R}$ with compact support contained in I, with $C_{c,+}^\infty(I)$ being the subclass of nonnegative functions. The Hilbert-Schmidt norm of an operator A is written as $\|A\|_2$, i.e., $\|A\|_2^2 = \operatorname{tr} A^*A$. $C_{a,b,\dots}$ will always denote some finite constant depending only on $a, b, \dots$.

A random Schrödinger operator H_ω shows dynamical localization in an open interval I if , with probability one, we have

$$\sup_{t\in\mathbb{R}} \big\| \langle X\rangle^{\frac{m}{2}} \mathrm{e}^{-itH_\omega} \mathscr{X}(H_\omega)\chi_0\,\varphi\big\| < \infty$$
$$\text{for all } \varphi \in \mathrm{L}^2(\mathbb{R}^d),\ \ \mathscr{X} \in C_{c,+}^\infty(I),\ \ m \geq 0. \tag{11}$$

But the known methods for proving Anderson localization also prove a stronger form of dynamical localization in a bounded open interval I, as follows:

- For the regular Anderson model (at the edges of the spectrum or for all energies for high disorder) and for the regular Anderson Hamiltonian (at the bottom of the spectrum), we have [4, 40, 6, 26, 41, 7, 70]

$$\mathbb{E}\Big\{\sup_{t\in\mathbb{R}}\big\|\langle X\rangle^{\frac{m}{2}}\mathrm{e}^{-itH_\omega}\mathscr{X}(H_\omega)\chi_0\big\|_2^2\Big\}<\infty \quad \text{for all } \mathscr{X}\in C^\infty_{c,+}(I),\ m\geq 0. \tag{12}$$

- For the Anderson Hamiltonian with μ arbitrary (e.g., a Bernoulli distribution) and for the Poisson Hamiltonian, given $0<s<\frac{3}{8}d$, at the bottom of the spectrum we have [47]

$$\mathbb{E}\Big\{\sup_{t\in\mathbb{R}}\big\|\langle X\rangle^{\frac{m}{2}}\mathrm{e}^{-itH_\omega}\mathscr{X}(H_\omega)\chi_0\big\|_2^{\frac{2s}{m}}\Big\}<\infty \quad \text{for all } \mathscr{X}\in C^\infty_{c,+}(I),\ m\geq 1. \tag{13}$$

5.2 Transport Exponents

To study dynamical delocalization it is convenient to introduce *transport exponents*. Let H_ω be a regular random Schrödinger operator, i.e., a regular Anderson model, Anderson Hamiltonian, or random Landau Hamiltonian. Following [45], we will measure the rate of growth of moments of initially spatially localized wave packets under the time evolution, localized in energy by $\mathscr{X}\in C^\infty_{c,+}(\mathbb{R})$ with $\mathscr{X}(H_\omega)\neq 0$, by the (lower) transport exponents ($m\geq 0$)

$$\beta(m,\mathscr{X}):=\liminf_{T\to\infty}\frac{\log\mathscr{M}(m,\mathscr{X},T)}{m\log T}, \tag{14}$$

where

$$\mathscr{M}(m,\mathscr{X},T):=\frac{1}{T}\int_0^{+\infty}\mathbb{E}\big\{M_\omega(m,\mathscr{X},t)\big\}\mathrm{e}^{-\frac{t}{T}}\,\mathrm{d}t, \tag{15}$$

with

$$M_\omega(m,\mathscr{X},t):=\big\|\langle X\rangle^{\frac{m}{2}}\mathrm{e}^{-itH_\omega}\mathscr{X}(H_\omega)\chi_0\big\|_2^2. \tag{16}$$

If $\mathscr{X}(H_\omega)=0$ we set $\beta_{B,\lambda}(m,\mathscr{X})=0$. Note that

$$\mathscr{M}(m,\mathscr{X},T)\gtrsim T^{m\,\beta(m,\mathscr{X})}\quad \text{as } T\to\infty. \tag{17}$$

We define the m-th *m-th local transport exponent* at the energy E by

$$\beta(m,E):=\lim_{\delta\to 0}\sup_{\mathscr{X}\in C^\infty_{c,+}(E-\delta,E+\delta)}\beta(m,\mathscr{X}). \tag{18}$$

These local transport exponents $\beta_{B,\lambda}(m,E)$ provide a measure of the rate of transport in wave packets with spectral support near E. They are increasing in m and hence we define the *local asymptotic transport exponent* at E by

$$\beta(E):=\lim_{m\to\infty}\beta(m,E)=\sup_{m>0}\beta(m,E). \tag{19}$$

Transport exponents have the following properties [45]:

- $0\leq\beta(m,E)\leq 1$, increasing in $m\Rightarrow 0\leq\beta(E)\leq 1$.

- $\beta(E) > 0 \Leftrightarrow \beta(m, E) > 0$ for some $m > 0$.
- $E \notin \Sigma \Rightarrow \beta(E) = 0$.

5.3 The Dynamical Spectral Regions

We will say that the regular random Schrödinger operator H_ω exhibits *dynamical localization* at the energy E if (12) holds in some interval of the form $(E-\delta, E+\delta)$, which we can rewrite as

$$\mathbb{E}\Big\{\sup_{t\in\mathbb{R}} M_\omega(m, \mathscr{X}, t)\Big\} < \infty \quad \text{for all } \mathscr{X} \in C^\infty_{c,+}((E-\delta, E+\delta)) \text{ and } m \geq 0. \tag{20}$$

It follows immediately that if H_ω exhibits dynamical localization at the energy E we must have $\beta(E) = 0$.

On the other hand, it follows from Guarneri's bound [56, 57, 19, 79] that the absolutely continuous spectrum Σ_{ac} of H_ω satisfies

$$\Sigma_{ac} \subset \Big\{E \in \mathbb{R};\ \beta(E) \geq \frac{1}{d}\Big\}. \tag{21}$$

(Note that the converse is not true, a lower bound on the local transport exponent does not specify the spectrum, cf. [31, 79, 28, 12, 22, 48].)

These considerations motivate the definition of two complementary regions in the energy axis (cf. [45], note that different names are used in that paper):

- The *region of dynamical localization*:

$$\Xi^{\mathrm{DL}} := \{E \in \mathbb{R};\quad \beta(E) = 0\}.$$

- The *region of dynamical delocalization*:

$$\Xi^{\mathrm{DD}} := \{E \in \mathbb{R};\quad \beta(E) > 0\}.$$

In addition, an energy $\tilde{E} \in \Xi^{\mathrm{DD}} \cap \{\overline{\Xi^{DL} \cap \Sigma}\}$ will be called a *dynamical mobility edge*. Note that:

- Ξ^{DL} is an open set, and hence Ξ^{DD} is a closed set.
- $\Xi^{\mathrm{DD}} \subset \Sigma$, and hence $\mathbb{R} \setminus \Sigma \subset \Xi^{\mathrm{DL}}$.

These definitions are justified by the following characterization of the dynamical spectral regions.

Theorem 1 ([45]). *Let H_ω be a regular random Schrödinger operator. Then*

$$\Xi^{\mathrm{DL}} = \{E \in \mathbb{R};\ H_\omega \text{ exhibits dynamical localization at } E\} \tag{24}$$

and

$$\Xi^{\mathrm{DD}} = \Big\{E \in \mathbb{R};\ \beta(E) \geq \frac{1}{2d}\Big\}. \tag{25}$$

Moreover, H_ω exhibits Anderson localization in Ξ^{DL} and the absolutely continuous spectrum $\Sigma_{ac} \subset \Xi^{\mathrm{DD}}$.

This theorem follows from the fact that slow transport cannot occur for regular random Schrödinger operators.

Theorem 2 ([45]). *Let H_ω be a regular random Schrödinger operator. Let $\mathscr{X} \in C^\infty_{c,+}(\mathbb{R})$, with $\mathscr{X} \equiv 1$ on some open interval I, $\alpha \geq 0$, and $m > 2d\alpha + 11d$. If*

$$\liminf_{T\to\infty} \frac{1}{T^\alpha} \mathscr{M}(m, \mathscr{X}, T) < \infty, \tag{26}$$

then $I \subset \Xi^{\mathrm{DL}}$.

5.4 The Region of Complete Localization

Let H_ω be a regular random Schrödinger operator. The region of dynamical localization Ξ^{DL} has a large number of very natural properties, all equivalent to the definition [45]. There is an appealing analogy with classical statistical mechanics: the energy is the parameter that corresponds to the temperature, the region of Anderson localization is the analogous concept to the single phase region with exponentially decaying correlation functions, and Ξ^{DL} corresponds to the region of complete analyticity [33, 34], possessing every possible virtue we can imagine! For this reason Ξ^{DL} is also called the *region of complete localization* [46, 24]. In particular, we have the following characterization in terms of the decay of the Fermi projections $P^{(E)}_\omega := \chi_{]-\infty,E]}(H_\omega)$. Recall that Ξ^{DL} is an open subset of $\mathbb{R}$.

Theorem 3 ([46]). *Let H_ω be a regular random Schrödinger operator and I a bounded open interval. Then*

1. *If $I \subset \Xi^{\mathrm{DL}}$, for all $\zeta \in]0,1[$ there is a constant $C_{I,\zeta}$ such that*

$$\mathbb{E}\Big\{ \sup_{E\in I} \big\| \chi_x P^{(E)}_\omega \chi_y \big\|_2^2 \Big\} \leq C_{I,\zeta}\, \mathrm{e}^{-|x-y|^\zeta} \quad \text{for all } x, y \in \mathbb{Z}^d. \tag{27}$$

2. *If for some $\zeta \in]0,1[$ (27) holds with some constant $C_{I,\zeta}$, then $I \subset \Xi^{\mathrm{DL}}$. (It suffices to have sufficient polynomial decay in (27)).*

Moreover, when $I \subset \Xi^{\mathrm{DL}}$ the following holds with probability one:

- *H_ω has pure point spectrum in I.*
- *For all $\varepsilon > 0$ there are constants $m_{I,\varepsilon} > 0$ and $C_{I,\varepsilon,\omega}$ such that for all eigenfunctions ψ, φ of H_ω with the same eigenvalue $E \in I$, setting $\|\psi\|_- := \|\langle X\rangle^{-d}\psi\|$, we have*

$$\|\chi_x\psi\|\, \|\chi_y\varphi\| \leq C_{I,\varepsilon,\omega} \|\psi\|_- \|\varphi\|_- \, \mathrm{e}^{(\log\langle y\rangle)^{1+\varepsilon}} \mathrm{e}^{-m_\varepsilon|x-y|}.$$

- *The eigenvalues of H_ω in I have finite multiplicity.*

6 The Dynamical Transition in the Random Landau Hamiltonian

Explanations of the quantum Hall effect assume that under weak disorder and strong magnetic field the energy spectrum of the random Landau Hamiltonians consists of bands of extended states separated by energy regions of localized states and/or energy gaps [80, 58, 95, 76, 14]. This transition is not expected to be the spectral metal-insulator transition described in Sect. 4; the extend states may be due to singular continuous spectrum or delocalization may occur at a single energy [95]. But the assumption under these explanations has been validated by a proof of the occurrence of the dynamical metal-insulator transition in each spectral band of the random Landau Hamiltonian [52].

The random Landau Hamiltonian, introduced in Sect. 2.3, is given by

$$H_{B,\lambda,\omega} = H_B + \lambda V_\omega \quad \text{on} \quad \mathrm{L}^2(\mathbb{R}^2),$$

where H_B, given in (7), is the (free) Landau Hamiltonian, $\lambda > 0$ is the disorder parameter, and V_ω is the random potential in (6). We will assume that $H_{B,\lambda,\omega}$ is regular, i.e., the common probability distribution μ has a bounded density ρ, and that ρ has support in the bounded interval $[-M_1, M_2]$ $(0 \le M_1, M_2 < \infty, M_1 + M_2 > 0)$. Without loss of generality we set $\|\sum_{i\in\mathbb{Z}^2} u(x-i)\|_\infty = 1$, so $-M_1 \le V_\omega(x) \le M_2$.

The spectrum $\sigma(H_B)$ of the Landau Hamiltonian H_B consists of a sequence of infinitely degenerate eigenvalues, the Landau levels:

$$B_n = (2n-1)B, \quad n = 1, 2, \ldots. \tag{29}$$

It is convenient to set $B_0 = -\infty$. A simple argument shows that

$$\Sigma_{B,\lambda} \subset \bigcup_{n=1}^{\infty} \mathscr{B}_n(B,\lambda), \quad \text{where } \mathscr{B}_n(B,\lambda)[B_n - \lambda M_1, B_n + \lambda M_2]. \tag{30}$$

If the *disjoint bands condition*

$$\lambda(M_1 + M_2) < 2B, \tag{31}$$

is satisfied (true at either weak disorder or strong magnetic field), the (disorder-broadened) Landau bands $\mathscr{B}_n(B,\lambda)$ are disjoint, and hence the open intervals

$$\mathscr{G}_n(B,\lambda) =]B_n + \lambda M_2, B_{n+1} - \lambda M_1[, \quad n = 0, 1, 2, \ldots, \tag{32}$$

are nonempty spectral gaps for $H_{B,\lambda,\omega}$. Moreover, if $\rho > 0$ a.e. on $[-M_1, M_2]$ and (31) holds, then for each $B > 0$, $\lambda > 0$, and $n = 1, 2, \ldots$ there are $a_{j,B,\lambda,n} \in [0, \lambda M_j]$, $j = 1, 2$, continuous in λ, such that, by an argument of [61],

$$\Sigma_{B,\lambda} \bigcup_{n=1}^{\infty} \mathscr{I}_n(B,\lambda), \quad \text{where } \mathscr{I}_n(B,\lambda)[B_n - a_{1,B,\lambda,n}, B_n + a_{2,B,\lambda,n}]. \tag{33}$$

The existence of dynamical delocalization is given in the following theorem.

Theorem 4 ([52]). *The random Landau Hamiltonian $H_{B,\lambda,\omega}$ under the disjoint bands condition (31) exhibits dynamical delocalization in each band $\mathscr{B}_n(B,\lambda)$: for all $n = 1, 2, \ldots$ we have*

$$\Xi^{\mathrm{DD}}_{B,\lambda} \cap \mathscr{B}_n(B,\lambda) \neq \emptyset. \tag{34}$$

Thus there exists at least one energy $E_n(B,\lambda) \in \mathscr{B}_n(B,\lambda)$ such that

$$\beta_{B,\lambda}(E_n(B,\lambda)) \geq \frac{1}{4}. \tag{35}$$

In fact, for every $\mathscr{X} \in C^\infty_{c,+}(\mathbb{R})$ with $\mathscr{X} \equiv 1$ on some open interval $J \ni E_n(B,\lambda)$ and all $m > 0$ we have

$$\mathscr{M}_{B,\lambda}(m, \mathscr{X}, T) \geq C_{m,\mathscr{X}}\, T^{\frac{m}{4}-6} \tag{36}$$

for all $T \geq 0$ with $C_{m,\mathscr{X}} > 0$, and hence

$$\beta_{B,\lambda}(m, E_n(B,\lambda)) \geq \frac{1}{4} - \frac{6}{m} > 0 \quad \text{for all } m > 24. \tag{37}$$

Dynamical localization at the edges of the Landau bands for large magnetic field B has been known under mild hypotheses on u and μ [21, 99, 44]. In the regime of large magnetic field (and fixed disorder), we get the existence of the dynamical metal-insulator transition and of dynamical mobility edges for the model studied in [21, 44]. In fact, combining the results of [21, 44] with Theorem 4, we have the following rather complete picture, consistent with the prediction that at very large magnetic field there is only one delocalized energy in each Landau band, located at the Landau level [18].

Theorem 5 ([52]). *Consider a random Landau Hamiltonian $H_{B,\lambda,\omega}$ satisfying the following additional conditions on the random potential*: (i) $u \in C^2$ *and* $\operatorname{supp} u \subset D_{\frac{\sqrt{2}}{2}}(0)$, *the open disc of radius $\frac{\sqrt{2}}{2}$ centered at 0.* (ii) *The density of the probability distribution μ is an even function $\rho > 0$ a.e. on $[-M, M]$ ($M = M_1 = M_2$).* (iii) $\mu([0,s]) \geq c \min\{s, M\}^\zeta$ *for some $c > 0$ and $\zeta > 0$. Fix $\lambda > 0$ and let $B > 0$ satisfy (31), in which case the spectrum $\Sigma_{B,\lambda}$ is given by (33) with*

$$0 \leq \lambda M - a_{j,B,\lambda,n} \leq C_n(\lambda) B^{-\frac{1}{2}}, \quad j = 1, 2. \tag{38}$$

Then for each $n = 1, 2, \ldots$, if B is large enough (depending on n) there exist dynamical mobility edges $\widetilde{E}_{j,n}(B,\lambda)$, $j = 1, 2$, with

$$\max_{j=1,2} \left| \widetilde{E}_{j,n}(B,\lambda) - B_n \right| \leq K_n(\lambda) \frac{\log B}{B} \to 0 \quad \text{as } B \to \infty, \tag{39}$$

$$B_n - a_{1,B,\lambda,n} < \widetilde{E}_{1,n}(B,\lambda) \leq \widetilde{E}_{2,n}(B,\lambda) < B_n + a_{2,B,\lambda,n}, \tag{40}$$

$$[B_n - a_{1,B,\lambda,n}, \widetilde{E}_{1,n}(B,\lambda)[\cup]\widetilde{E}_{2,n}(B,\lambda), B_n + a_{2,B,\lambda,n}] \subset \Xi^{\mathrm{DL}}_{B,\lambda}. \tag{41}$$

(*By* $C_n(\lambda)$, $K_n(\lambda)$ *we denote finite constants. It is possible that* $\widetilde{E}_{1,n}(B,\lambda) \times \widetilde{E}_{2,n}(B,\lambda)$*, i.e., dynamical delocalization occurs at a single energy.*)

For extensions to more general random Landau Hamiltonians see [54, 53].

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Unifying R-Symmetry in M-Theory

Axel Kleinschmidt

Abstract In this contribution we address the following question: Is there a group with a fermionic presentation which unifies all the physical gravitini and dilatini of the maximal supergravity theories in $D = 10$ and $D = 11$ (without introducing new degrees of freedom)? The affirmative answer relies on a new mathematical object derived from the theory of Kac–Moody algebras, notably E_{10}. It can also be shown that in this way not only the spectrum but also dynamical aspects of all supergravity theories can be treated uniformly.

1 Introduction

One of the major themes in string theory has been unification. By this we mean that hitherto unrelated theories and their properties are interpreted as different aspects of a single more general and more fundamental model. In a very broad sense these advances can be called *duality relations* and typically were first largely conjectural but were substantiated later by computations. Among the most far-reaching of these duality conjectures is the M-theory conjecture [38, 19] which states that all five known superstring theories have a common origin which is usually termed M-theory. However, no complete definition of M-theory is known to date.

It is the aim of this contribution to illustrate how the M-theory picture can be made more precise by studying a somewhat restricted set-up. More precisely, we will focus on

- The low energy effective theories with maximal supersymmetry. These are the $D = 11$ supergravity theory and the $D = 10$ type IIA and type IIB theories.

Axel Kleinschmidt
Max Planck Institute for Gravitational Physics, Albert Einstein Institute, Am Mühlenberg 1, 14476 Potsdam, Germany, e-mail: axel.kleinschmidt@aei.mpg.de
Present address: Service de Physique Théorique et Mathématique, Université Libre de Bruxelles & International Solvay Instititutes, Campus Plaine CP231, Boulevard du Triomphe, 1050 Bruxelles, Belgium, e-mail: axel.kleinschmidt@ulb.ac.be

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- The fermionic sectors of these theories. Since all these models have maximal supersymmetry they have the same number of physical degrees of freedom, equal to 128, in their fermionic (and bosonic) sectors. However, these are distributed differently into representations of the relevant Lorentz and R-symmetries.

The fermionic spectra are summarised in Table 1. In that table, the relevant irreducible representations of the different Lorentz groups are indicated. Since a gravitino is a vector-spinor it always consists of a Γ-traceless part and a pure Γ-trace; in the $D = 11$ case these are the **320** and **32** respectively. As is well known, the type IIA theory employs spinors of both chiralities of the $D = 10$ Lorentz group whereas in type IIB only one chirality is used. The known relations for the various Lorentz groups following from dualities are:

$$\begin{array}{ccc} & SO_B(1,9) & \\ & \cup & \\ \cdots \subset & SO(1,8) & \subset SO_A(1,9) \subset SO(1,10) \end{array} \tag{1}$$

I.e. the type IIA theory is contained in the $D = 11$ theory (via dimensional reduction), but the type IIB theory is not. However, after reduction to $D = 9$ the IIA and IIB theories agree. The M-theory conjecture now stipulates that there be a unifying structure to this diagram. This is the first question we address here: *Is there a group K which has subgroups $SO(1,10)$, $SO_A(1,9)$ and $SO_B(1,9) \times SO(2)$ with embedding relations given as in* (1) *and with a spinor representation which decomposes under these subgroups into the representations of Table* 1? This *kinematical* question will be answered in the affirmative in Sect. 2.

The second question addressed in this contribution is: *Is there a dynamical equation with explicit K symmetry for the K spinor representation (constructed in the answer to the first question) which reduces to the dynamics of the fermionic fields of the various supergravity theories?* This *dynamical* question will receive a partially affirmative answer in Sect. 3.

The work reported on here is based on the papers [10, 13, 26, 11, 27] which studied the fermionic sectors of maximal supergravity theories and their symmetries.

Table 1 Fermionic representations of the various maximal supergravity theories in $D = 10$ and $D = 11$

Theory	Lorentz & R-symmetry	Representation
$D = 11$	$SO(1,10)$	Gravitino ψ_M
		$(\mathbf{320} \oplus \mathbf{32})$
$D = 10$ IIA	$SO_A(1,9)$	Two gravitini $\psi_\mu^{(1)}, \psi_\mu^{(1)}$ (achiral)
		$(\mathbf{144} \oplus \overline{\mathbf{16}}) \oplus (\overline{\mathbf{144}} \oplus \mathbf{16})$
		Two dilatini $\lambda^{(1)}, \lambda^{(2)}$ (achiral)
		$(\mathbf{16} \oplus \overline{\mathbf{16}})$
$D = 10$ IIB	$SO_B(1,9) \times SO(2)$	Two gravitini $\psi_\mu^{(1)}, \psi_\mu^{(1)}$ (chiral)
		$((\mathbf{144}, \mathbf{2}) \oplus (\overline{\mathbf{16}}, \mathbf{2}))$
		Two dilatini $\lambda^{(1)}, \lambda^{(2)}$ (chiral)
		$(\overline{\mathbf{16}}, \mathbf{2})$

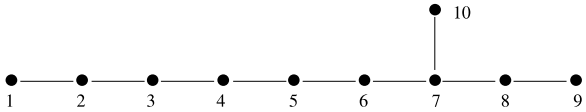


Fig. 1 Dynkin diagram of E_{10} with numbering of nodes. E_{11} has an additional node attached with a single line to node 1

The approach taken there (and also here) arises from known results of unifying symmetries in the corresponding bosonic sector. In particular, it was shown in [35, 33, 34, 8, 37, 31, 28] that the indefinite Kac–Moody algebras E_{10} and E_{11} contain the correct spectra at low levels in so-called level decompositions. The Dynkin diagram of E_{10} is given in Fig. 1 and the uncanny resemblance of the right end of the Dynkin diagram to the structure in (1) is not accidental. E_{11} contains the correct fields as covariant Lorentz tensor whereas E_{10} breaks Lorentz symmetry with only manifest spatial Lorentz symmetry.[1] The bosonic low level spectra correspond to the bosonic version of the first, kinematical question raised above—in order to address the second, dynamical question for bosons further 'specifications' are required. For E_{11}, West proposed in [35] that M-theory should be a non-linear realisation of E_{11}; if space-time also carries an E_{11} structure it nicely incorporates all central charges of the $D = 11$ supersymmetry algebra [36] but also infinitely many more new coordinates. The same E_{11} structure was found for the bosonic sectors of (massive) type IIA and type IIB in [35, 33, 34]. For E_{10}, Damour, Henneaux and Nicolai proposed in [8] a one-dimensional non-linear σ-model based on an E_{10} coset space and demonstrated that at low levels null geodesic motion on this coset space is equivalent to the $D = 11$ dynamics around a fixed spatial point truncated roughly after first spatial gradients. Higher order spatial gradients were conjectured to arise via the higher levels in the decomposition. This picture was extended to (massive) type IIA and type IIB in [23, 25]. A model combining E_{11} with the null geodesic idea of E_{10} was given in [16, 15].

In this contribution we will work with E_{10} because in this case we can give a more complete answer to the kinematical and dynamical questions raised above. Since E_{10} treats time and space asymmetrically, all necessary requirements for the sought-after 'M-theory Lorentz group' K only involve spatial Lorentz groups and their representations. We will comment on the covariant formulation in the final section. In order to convey the main ideas we mostly refrain from introducing intricate notations and outline the logic; more details can be found in references [10, 13, 26, 11].

[1] For this reason the level decomposition of E_{10} does not contain anti-symmetric ten-form fields for type IIA and type IIB [25] whereas E_{11} does [28]. That non-propagating ten-forms, as predicted by E_{11} are compatible with the supersymmetry algebra was verified in [1, 2].

2 Kinematics

The study of dimensional reduction [5, 6] suggests that the group K we are looking for is $K = K(E_{10})$, the 'maximal compact subgroup' of E_{10}. In order to see that this is true we first need to understand what $K(E_{10})$ is.

2.1 Definition of $\mathfrak{e}_{10}$ and $K(\mathfrak{e}_{10})$

$K(E_{10})$ is infinite-dimensional and since global issues are somewhat tricky we will restrict our attention here to the Lie algebras. The Lie algebra $K(\mathfrak{e}_{10})$ of $K(E_{10})$ is a subalgebra of the Lie algebra $\mathfrak{e}_{10}$ of E_{10}. The Lie algebra $\mathfrak{e}_{10}$ is defined in the Chevalley–Serre presentation by giving 30 simple generators

$$e_i, f_i, h_i \quad (i = 1, \ldots, 10) \tag{2}$$

and their relations (for all $i, j = 1, \ldots 10$)[2]

$$\begin{aligned} &[h_i, e_j] = A_{ij} e_j, \qquad [h_i, f_j] = -A_{ij} f_j, \qquad [e_i, f_j] = \delta_{ij} h_i, \\ &[h_i, h_j] = 0, \qquad (\mathrm{ad}\, e_i)^{1-A_{ij}} e_j = 0, \qquad (\mathrm{ad}\, f_i)^{1-A_{ij}} f_j = 0, \end{aligned} \tag{3}$$

where A_{ij} is the generalised Cartan matrix which can be read off from Fig. 1 as follows: $A_{ii} = 2$ for $i = 1, \ldots, 10$ and if there is a single link between nodes i and j then $A_{ij} = A_{ji} = -1$ and $A_{ij} = 0$ otherwise. $\mathfrak{e}_{10}$ is defined as the Lie algebra with simple generators (2) and relations (3).

On $\mathfrak{e}_{10}$ one can define the Chevalley involution θ acting by

$$\theta(e_i) = -f_i, \qquad \theta(f_i) = -e_i, \qquad \theta(h_i) = -h_i \tag{4}$$

on the simple generators. The fixed point set of this involution defines the 'compact subalgebra' $K(\mathfrak{e}_{10})$:

$$K(\mathfrak{e}_{10}) = \{x \in \mathfrak{e}_{10} : \theta(x) = x\}. \tag{5}$$

This subalgebra is called compact because it has definite Killing norm, generalising the notion of compact algebras in the finite-dimensional case.

It can be shown [3] that $K(\mathfrak{e}_{10})$ is generated by the simple generators

$$x_i = e_i - f_i \quad (i = 1, \ldots, 10) \tag{6}$$

which are manifestly invariant under θ and defining relations of the type

$$\sum_{k=0}^{1-A_{ij}} C_{ij}^{(k)} (\mathrm{ad}\, x_i)^k x_j = 0, \tag{7}$$

[2] ad denotes the adjoint action: $(\mathrm{ad}\, e_i) e_j = [e_i, e_j]$.

where $C_{ij}^{(k)}$ are constant coefficients and can be computed from the Cartan matrix. This defines a presentation of $K(\mathfrak{e}_{10})$ in terms of generators and relations. For both $\mathfrak{e}_{10}$ and $K(\mathfrak{e}_{10})$ this type of presentation is the only known presentation. Whereas $\mathfrak{e}_{10}$ is a Kac–Moody algebra with well-defined structure theory [21], $K(\mathfrak{e}_{10})$ is *not* a Kac-Moody algebra [24] and its general representation theory is unknown. Nevertheless, the relations (7) are sufficient to establish the consistency of any tentative representation as we will see below. All Lie algebras we consider are over the real numbers, in particular $\mathfrak{e}_{10}$ is in split form.

2.2 Level Decompositions for $D = 11$, IIA and IIB

A more economical and physical description of the generators of $\mathfrak{e}_{10}$ can be obtained via a so-called level decomposition [8, 28] where one represents

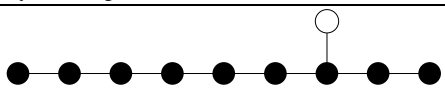
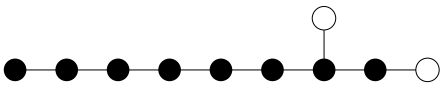
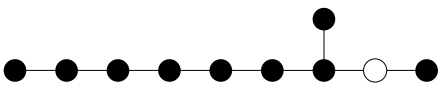
$$\mathfrak{e}_{10} = \sum_{\ell \in \mathbb{Z}} \mathfrak{e}_{10}^{(\ell)} \tag{8}$$

as a graded sum of (finite-dimensional reducible) representation spaces of a chosen regular subalgebra. The subalgebras of interest are obtained by removing nodes from the E_{10} Dynkin diagram. The integer ℓ represents the level (if several nodes are removed it consists of a tuple of integers). Regular subalgebras of $\mathfrak{e}_{10}$ naturally give rise to subalgebras of $K(\mathfrak{e}_{10})$.

The subalgebras relevant for $D = 11$, type IIA and type IIB are displayed in Table 2. From the table it is evident that $K(\mathfrak{e}_{10})$ admits subalgebras of the type required by condition (1) and that these satisfy the necessary embedding conditions. (Recall that the time coordinate is treated separately for E_{10} whence we are only dealing with the spatial Lorentz groups here.)

We exemplify the result of the level decomposition for the $D = 11$ case, that is for the case of the depicted $\mathfrak{sl}(10)$ subalgebra of $\mathfrak{e}_{10}$. At level $\ell = 0$ the reducible representation of $\mathfrak{sl}(10)$ turns out to be $\mathfrak{gl}(10)$ with generators $K^a{}_b$. Moreover, all

Table 2 The subalgebras relevant for the various maximal supergravity theories. Empty nodes are to be deleted

Theory	Dynkin diagram	Subalgebra of $\mathfrak{e}_{10}$	... of $K(\mathfrak{e}_{10})$
$D = 11$		$\mathfrak{sl}(10)$	$\mathfrak{so}(10)$
$D = 10$ IIA		$\mathfrak{sl}_A(9)$	$\mathfrak{so}_A(9)$
$D = 10$ IIB		$\mathfrak{sl}_B(9) \oplus \mathfrak{sl}(2)$	$\mathfrak{so}_B(9) \oplus \mathfrak{so}(2)$

higher levels are representations of $\mathfrak{gl}(10)$. Concretely,

$$\begin{aligned}
&\ell = 0 : K^a{}_b \\
&\ell = 1 : E^{abc} = E^{[abc]} \\
&\ell = 2 : E^{a_1\ldots a_6} = E^{[a_1\ldots a_6]} \\
&\ell = 3 : E^{a_0|a_1\ldots a_8} = E^{a_0|[a_1\ldots a_8]}, \qquad E^{[a_0|a_1\ldots a_8]} = 0 \\
&\quad\vdots \qquad\quad \vdots
\end{aligned} \tag{9}$$

Here, $(a, b = 1, \ldots, 10)$ are $\mathfrak{sl}(10)$ vector indices and $\ell = 1, 2, 3$ are irreducible representations (accidentally). These tensors suggest a relation to the bosonic fields of $D = 11$ as follows: $\ell = 0$ is related to the spatial part $e_m{}^a$ of the vielbein, $\ell = 1$ is related to the spatial components of the anti-symmetric three-form gauge potential, $\ell = 2$ is related to the Hodge dual of the three-form potential and $\ell = 3$ is related to the dual of the vielbein. That this is true in the one-dimensional $E_{10}/K(E_{10})$ σ-model was shown in [8].

Our interest here is in $K(E_{10})$ and therefore we have to form the invariant combinations of the generators in (9) to obtain

$$\begin{aligned}
&\ell = 0 : J^{ab} = K^a{}_b + \theta(K^a{}_b) = K^a{}_b - K^b{}_a = J^{[ab]} \\
&\ell = 1 : J^{abc} = E^{abc} + \theta(E^{abc}) \\
&\ell = 2 : J^{a_1\ldots a_6} = E^{a_1\ldots a_6} + \theta(E^{a_1\ldots a_6}) \\
&\ell = 3 : J^{a_0|a_1\ldots a_8} = E^{a_0|a_1\ldots a_8} + \theta(E^{a_0|a_1\ldots a_8}) \\
&\quad\vdots \qquad\quad \vdots
\end{aligned} \tag{10}$$

For $K(\mathfrak{e}_{10})$ the level ℓ has to be taken with a grain of salt since it does no longer define a grading but only a filtered structure. Indeed, examples of $K(\mathfrak{e}_{10})$ commutation relations are [10]

$$\begin{aligned}
[J^{ab}, J^{cd}] &= \delta^{bc} J^{ad} - \delta^{bd} J^{ac} - \delta^{ac} J^{bd} + \delta^{ad} J^{bc}, \\
[J^{a_1a_2a_3}, J^{a_4a_5a_6}] &= J^{a_1\ldots a_6} - 18\delta^{[a_1a_2}_{[a_4a_5} J^{a_3]}{}_{a_6]}.
\end{aligned} \tag{11}$$

We see that the first line is the $\mathfrak{so}(10)$ subalgebra of $K(\mathfrak{e}_{10})$ and the second line gives generators of 'levels' $\ell = 2$ and $\ell = 0$ on the right hand side in accordance with the filtered structure. The $\mathfrak{so}(10)$ subalgebra introduces the invariant δ^{ab} which can be used to raise and lower the tensor indices. There are infinitely many more relations than (11) involving all the other infinitely many generators and no closed form is known for them.

2.3 Representations of $K(\mathfrak{e}_{10})$

By virtue of the presentation of $K(\mathfrak{e}_{10})$ in terms of generators and relations in (6) and (7) it is sufficient to verify a finite number of relations on a tentative representa-

tion. Using the level decomposition one can further reduce this number by starting from a representation of the subalgebra (which obviously constitutes a necessary condition). Then the sufficient consistency conditions involve only levels $\ell = 0$ and $\ell = 1$ (basically since there are only single lines in the E_{10} Dynkin diagram). For the $\mathfrak{so}(10)$ subalgebra of $K(\mathfrak{e}_{10})$ the recipe for constructing $K(\mathfrak{e}_{10})$ representations is:

1. Start from an $\mathfrak{so}(10)$ representation which we call the tentative $K(\mathfrak{e}_{10})$ representation. This defines the action of the J^{ab} generators within $K(\mathfrak{e}_{10})$ on the tentative representation.
2. Make a general ansatz for the action of J^{abc} on the tentative representation from $\mathfrak{so}(10)$ representation theory.
3. Verify that the second line of (11) holds for the case when some of indices are identical on the tentative representation. When some indices are identical the term with six anti-symmetric indices drops out.[3] If there is a solution for the general ansatz then the tentative representation gives rise to a full consistent representation of $K(\mathfrak{e}_{10})$.

For the other subalgebras the procedures are similar. Since it involves the tensors arising in the corresponding level decompositions we do not detail them here in order to keep the exposition simple.

We now construct the gravitino (vector-spinor) representation of $K(\mathfrak{e}_{10})$ following the steps above. The vector-spinor of $\mathfrak{so}(10)$ is reducible of dimension 320 and consists of the irreducible pieces $\mathbf{288} \oplus \mathbf{32}$ corresponding to the Γ-traceless part and the Γ-trace. We denote the vector-spinor by ψ_a and suppress the spinor index. The $\mathfrak{so}(10)$ generators J^{ab} act on ψ_a by[4]

$$J^{ab}\psi_c = \frac{1}{2}\Gamma^{ab}\psi_c + 2\delta_c^{[a}\psi^{b]}. \tag{12}$$

In the general ansatz for the J^{abc} action there are three terms and the solution to the necessary commutation condition (11) leads to [10, 13]

$$J^{abc}\psi_d = \frac{1}{2}\Gamma^{abc}\psi_d + 4\delta_d^{[a}\Gamma^b\psi^{c]} - \Gamma_d{}^{[ab}\psi^{c]}. \tag{13}$$

That there exists a solution to the consistency condition implies that there is a representation of $K(\mathfrak{e}_{10})$ of dimension 320. One can check that this is in fact an irreducible representation since the Γ-trace no longer separates once J^{abc} is considered. *We have thus proved that* $K(\mathfrak{e}_{10})$ *has an irreducible* **320** *representation*. Under the $\mathfrak{so}(10)$ subalgebra it decomposes according to

$$\begin{array}{ccc} \mathbf{320} & \longrightarrow & \mathbf{288} \oplus \mathbf{32} \\ K(\mathfrak{e}_{10}) & \supset & \mathfrak{so}(10) \end{array} \tag{14}$$

[3] That this is sufficient follows from the precise expressions for the simple $K(\mathfrak{e}_{10})$ generators x_i of (6) in terms of components of the J^{ab} and J^{abc} which can be found in [11].

[4] Here, Γ^a are the real (32×32) $SO(10)$ Γ-matrices and $\Gamma^{ab} = \Gamma^{[a}\Gamma^{b]}$ etc.

as required. We denote this representation by Ψ since it can be defined independently of the $\mathfrak{so}(10)$ subalgebra under which it is more conveniently written as ψ_a.

We now turn to the decompositions under the subalgebras relevant for type IIA and type IIB. They were derived in [26] and we reproduce the results here as[5]

$$\begin{array}{ccc} \mathbf{320} & \longrightarrow & (\mathbf{128} \oplus \mathbf{16}) \oplus (\mathbf{128} \oplus \mathbf{16}) \oplus \mathbf{16} \oplus \mathbf{16} \\ K(\mathfrak{e}_{10}) & \supset & \mathfrak{so}_A(9) \end{array} \tag{15}$$

for type IIA, where the last two **16**s are the dilatini, and

$$\begin{array}{ccc} \mathbf{320} & \longrightarrow & ((\mathbf{128}, \mathbf{2}) \oplus (\mathbf{16}, \mathbf{2})) \oplus (\mathbf{16}, \mathbf{2}) \\ K(\mathfrak{e}_{10}) & \supset & \mathfrak{so}_B(9) \oplus \mathfrak{so}(2) \end{array} \tag{16}$$

for type IIB. Here, the last doublet of **16**s corresponds to the IIB dilatini. Since we are only dealing with the spatial Lorentz group $\mathfrak{so}(9)$ different chiralities are not properly distinguished. The calculation shows, however, that the two doublets of **16**s arise differently and in the covariant calculation one can show that indeed all chiralities also fulfill the necessary requirements to answer the first question raised in the introduction affirmatively: The group $K(E_{10})$ contains the subalgebras required by the M-theory picture and has a spinorial representation with the correct number of components which branches correctly to the fermionic fields of the maximal supergravity theories.

3 Dynamics

To further substantiate the significance of $K(E_{10})$ and its **320** representation Ψ for an algebraic approach to M-theory we now turn to studying a dynamical equation for Ψ and its relation to the fermionic dynamics in the various maximal supergravities.

Since time is treated separately in the E_{10} context and all dynamical equations in the bosonic sector are time evolution equations a natural ansatz for the fermionic equation is

$$\mathscr{D}_t \Psi = 0. \tag{17}$$

This is a Dirac equation for the $K(\mathfrak{e}_{10})$ vector-spinor coupled minimally to a $K(\mathfrak{e}_{10})$ connection $\mathscr{Q}_t$ via the covariant derivative

$$\mathscr{D}_t = \partial_t - \mathscr{Q}_t, \tag{18}$$

where $\mathscr{Q}_t \in K(\mathfrak{e}_{10})$ acts on Ψ in the **320** representation. The gauge field $\mathscr{Q}_t$ transforms under t-dependent local $K(E_{10})$ gauge transformations. As an $K(\mathfrak{e}_{10})$ ele-

[5] In [26] the subalgebra $\mathfrak{so}(9,9)$ was chosen for type IIA (instead of $\mathfrak{sl}_A(9)$) since this more naturally includes the mass term of the massive extension of IIA. That the result given here is also correct follows immediately from $\mathfrak{so}_A(9) \subset \mathfrak{so}(10)$ and the branching rules for these groups.

ment, $\mathscr{Q}_t$ can be expanded over $\mathfrak{so}(10)$ in the generators (10) via

$$\mathscr{Q}_t = \frac{1}{2} Q^{(0)}_{ab} J^{ab} + \frac{1}{3!} Q^{(1)}_{abc} J^{abc} + \frac{1}{6!} Q^{(2)}_{a_1 \dots a_6} J^{a_1 \dots a_6} + \frac{1}{9!} Q^{(3)}_{a_0 | a_1 \dots a_8} J^{a_0 | a_1 \dots a_8} + \cdots . \tag{19}$$

Since the action of all the $K(\mathfrak{e}_{10})$ generators can be computed from multiple commutators of (12) and (13) the Dirac equation (17) can be evaluated to arbitrary level. In [10] it was evaluated up to $\mathfrak{sl}(10)$ level three which is the level to which the field content (9) is understood [8]. The resulting expression contains the gauge field components $Q^{(\ell)}$ (for $\ell = 0, \dots, 3$) contracted with various Γ-matrices multiplying the $\mathfrak{so}(10)$ decomposed vector-spinor $\Psi = (\psi_a)$. Explicitly, we find

$$\begin{aligned} \mathscr{D}_t \psi_c = {} & \partial_t \psi_c - \frac{1}{4} Q^{(0)}_{ab} \Gamma^{ab} \psi_c - Q^{(0)}_{ca} \psi^a - \frac{1}{12} Q^{(1)}_{a_1 a_2 a_3} \Gamma^{a_1 a_2 a_3} \psi_c \\ & - \frac{2}{3} Q^{(1)}_{c a_1 a_2} \Gamma^{a_1} \psi^{a_2} + \frac{1}{6} Q^{(1)}_{a_1 a_2 a_3} \Gamma_c{}^{a_1 a_2} \psi^{a_3} - \frac{1}{1440} Q^{(2)}_{a_1 \dots a_6} \Gamma^{a_1 \dots a_6} \psi_c \\ & + \frac{1}{72} Q^{(2)}_{c a_1 \dots a_5} \Gamma^{a_1 \dots a_4} \psi^{a_5} - \frac{1}{180} Q^{(2)}_{a_1 \dots a_6} \Gamma_c{}^{a_1 \dots a_5} \psi^{a_6} \\ & - \frac{2}{3 \cdot 8!} Q^{(3)}_{a_0 | a_1 \dots a_8} \Gamma_c{}^{a_1 \dots a_8} \psi^{a_0} - \frac{2}{3 \cdot 7!} Q^{(3)}_{c | a_1 \dots a_8} \Gamma^{a_1 \dots a_7} \psi^{a_8} \\ & - \frac{4}{3 \cdot 8!} Q^{(3)}_{b | b a_1 \dots a_7} \Gamma^{a_1 \dots a_7} \psi_c - \frac{1}{3 \cdot 6!} Q^{(3)}_{b | b a_1 \dots a_7} \Gamma_c{}^{a_1 \dots a_6} \psi^{a_7} + \cdots . \end{aligned} \tag{20}$$

This equation has to be compared with the dynamical equation for the gravitino in $D = 11$ supergravity. From the analysis of the bosonic sector it is to be expected that gauge-fixing is required in order to establish a connection between the $K(\mathfrak{e}_{10})$ equation (20) and the supergravity equation [24]. Indeed it turns out [10] that one has to fix a supersymmetry gauge ($\psi_0 - \Gamma_0 \Gamma^a \psi_a = 0$) for the fermions, a pseudo-Gaussian gauge ($E_t{}^a = 0$) for the vielbein and a Coulomb gauge ($A_{0ab} = 0$) for the gauge potential. In this case the supergravity equation (to lowest fermion order) takes almost the same form as (20) but where the gauge field components take the values [10, 11]

$$\begin{aligned} Q^{(0)}_{ab}(t) &= -N \omega_{0\,ab}(t, \mathbf{x}_0), & Q^{(2)}_{a_1 \dots a_6}(t) &= -\frac{1}{4!} N \epsilon_{a_1 \dots a_6 b_1 \dots b_4} F_{b_1 \dots b_4}(t, \mathbf{x}_0), \\ Q^{(1)}_{abc}(t) &= N F_{0abc}(t, \mathbf{x}_0), & Q^{(3)}_{a_0 | a_1 \dots a_8}(t) &= \frac{3}{2} N \epsilon_{a_1 \dots a_8 b_1 b_2} \omega_{b_1\,b_2 a_0}(t, \mathbf{x}_0). \end{aligned} \tag{21}$$

Here, $\omega_{0\,ab}$ and $\omega_{a\,bc}$ are 'electric' and 'magnetic' components of the spin connection in flat indices; similarly F_{0abc} and $F_{b_1 \dots b_4}$ are electric and magnetic components of the four-form field strength in flat indices. The lapse $N = E_t{}^0$ is needed to convert the objects on the right hand sides into components of a world-line tensor $\mathscr{Q}_t$.

The equations (21) are valid only at a fixed spatial point $\mathbf{x}_0$ and in order to match (20) to the supergravity equation higher spatial gradients of the fields (and the lapse) have to be ignored. Furthermore, the spatial spin connection must have vanishing trace $\omega_{b\,ba} = 0$ at $\mathbf{x}_0$. More details can be found in [10, 11].

To summarise, with the use of the 'dictionary' (21) we have succeeded in turning a truncated version of the $D = 11$ gravitino equation of motion into a $K(E_{10})$ covariant Dirac-equation of the type (17). Although not explicitly proved in the type IIB case, one can expect that the very same equation (17) also describes the correct fermionic dynamics of type IIA and IIB by using the decompositions of $K(\mathfrak{e}_{10})$ detailed in (15) and (16).

Thus we arrive at the main result: $K(E_{10})$ is not only a viable candidate for a kinematical unification of the fermionic symmetries of *all* maximal supergravity theories but also can partially be established as a symmetry of the dynamical equations for the fermions.

4 Discussion

4.1 Remarks

Here, we only briefly sketch some related points and comment on a fully covariant reformulation of the above results.

There exists also a **32** representation of $K(\mathfrak{e}_{10})$ which was called 'Dirac-spinor' in [12, 10]. This representation is relevant for the supersymmetry parameter ϵ and similarly has the correct branching to the various maximal supergravity theories' Lorentz and R-symmetries [26].

Both the **320** and the **32** representations of $K(\mathfrak{e}_{10})$ are *unfaithful* since they are finite-dimensional representations of an infinite-dimensional algebra. This implies that $K(\mathfrak{e}_{10})$ is not a simple Lie algebra but has non-trivial quotients. These one arrives at by factoring out the ideals associated with the unfaithful representations [11]. In the case of the **32** Dirac-spinor the quotient is $\mathfrak{so}(32)$ which has been conjectured as a *generalised holonomy* in [14, 18]. Since $K(E_{10})$ acts not only on the Dirac-spinor but also on the **320** gravitino (which $SO(32)$ does not) it is more general than these conjectured holonomies. Furthermore, certain global issues [22] are resolved in $K(E_{10})$ [10].

As mentioned in the introduction, the M-theoretic properties of $K(E_{10})$ were derived following similar results in the bosonic sector [35, 33, 34, 8, 23, 25]. The bosonic fields are realised via a coset construction $E_{10}/K(E_{10})$ where $K(E_{10})$ also acts as a local gauge symmetry. It is non-trivial, but true, that the relation between the gauge connection appearing in the bosonic analysis and the one in the fermionic analysis are related in precisely the same way to the supergravity quantities via (21).

It can also be shown that $K(E_{11})$ (if equipped with the temporal involution of [16]) allows for a fermionic representation of dimension $352 = 320 + 32$ if written

over $SO(1,10)$ [26]. The IIA and IIB decompositions of this fully covariant gravitino give the correct achiral and chiral fermionic spectra in a covariant fashion so that all the results of Sect. 2 carry over to $K(E_{11})$. However, it is not clear how to write a $K(E_{11})$ covariant and space-time covariant dynamical equation for this gravitino which generalises the Dirac equation (17). An obvious candidate is

$$\not{\mathscr{D}}\Psi = 0, \tag{22}$$

where $\not{\mathscr{D}} = \Gamma^M \mathscr{D}_M = \Gamma^M(\partial_M - \mathscr{Q}_M)$. There are a number of subtleties with this suggestive notation that need to be clarified. Firstly, $\mathscr{D}_M$ should be $K(E_{11})$ covariant meaning that the gauge fields transform correctly under $K(E_{11})$. By augmenting an $E_{11}/K(E_{11})$ coset construction by a Borisov–Ogievetsky type construction as in [35] this can probably be achieved. The second problematic point is the symbol Γ^M used above since Γ^M is not an $K(E_{11})$ invariant tensor and so spoils the $K(E_{11})$ covariance of the equation even if $\mathscr{D}_M$ transforms correctly. In line with the philosophy of [36] one should probably replace eleven-dimensional space-time indices M by indices taking values in an infinite-dimensional highest weight representation of E_{11} generalising the translation vector to an E_{11} object. It remains to be seen whether one can make sense of (22) in this framework.

4.2 Outlook

From the discussion in the introduction it is clear that in order to complete the M-theory picture a number of things need to be included in the present algebraic framework, the most pressing of which we briefly discuss now.

Firstly, M-theory should also include the non-maximal heterotic $E_8 \times E_8$ and $SO(32)$ string theories as well as the $SO(32)$ type I superstring. At low energies this requires fitting the heterotic $D = 10$ supergravity with gauge groups $SO(32)$ and $E_8 \times E_8$ into the E_{10} σ-model or some more general model. As a first step it was shown in [23, 17] that the pure type I supergravity (without any vector multiplets) can be interpreted as a subsector of the E_{10} model. It would be gratifying to see a relation between the algebraic approach taken here and the issue of anomaly freedom.

Secondly, M-theory presumably is a theory of strings and other extended objects. The analysis so far only covered point particles since properties of the low energy field theories were studied. It is not clear if the symmetries found need to be modified when extended objects are also considered. Results from U-duality [19, 32] suggest that the continuous symmetry gets broken to some discrete arithmetic group and first ideas in this direction were discussed in [4]. A different route was taken in [7, 9] where string induced higher derivative corrections to the low energy effective action were studied in relation to E_{10} and good agreement between the algebraic structure and conjectured properties of these correction terms was found (see also [29]).

Thirdly, the bosonic fields appear through the infinite—dimensional coset space $E_{10}/K(E_{10})$ whereas the fermionic fields presently are confined to a finite—dimensional, unfaithful representation of $K(E_{10})$. This seems problematic from a supersymmetry point of view. This dichotomy is partly related to the difference in order of the equations of motion for bosons and fermions. The fermionic field equations are first order whereas the bosonic ones are second order (allowing for dualisations and triggering for example the infinite duality cascade in $D = 2$). It would be nice to overcome this obstacle through the construction of an appropriate faithful fermionic representation of $K(E_{10})$.

Finally, on the purely mathematical side it could be hoped that a proper understanding of the relation between E_{10} and M-theory may lead to a new presentation of the E_{10} structure itself. Since its inception in the late 1960s [20, 30] the theory of indefinite Kac–Moody algebras has produced few results which truly penetrate the structure of these fascinating objects.

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Stable Maps are Dense in Dimensional One

Oleg Kozlovski, and Sebastian van Strien

Abstract This is an exposition of our resent results contained in Kozlovski et al. (Rigidity for real polynomials, preprint, 2003; Density of hyperbolicity, preprint, 2003) and Kozlovski and van Strien (Local connectivity and quasi-conformal rigidity of non-renormalizable polynomials, preprint, 2006) where we prove the density of hyperbolicity for one dimensional real maps and non-renormalizable complex polynomials. The proofs of these results are very technical, so in this paper we try to show the main ideas on some simplified examples and also give some outlines of the proofs.

1 Introduction

One of the central aims in dynamical systems is to describe dynamics of a 'typical' system. In this article we will understand the word 'typical' from the topological point of view.

The nicest kind of system is one which is stable (also called *structurally stable*): this means that it is topologically conjugate to any sufficiently nearby system. This notion is closely related to that of hyperbolicity of the system (see below).

The most ambitious hope would be to show that structurally stable and hyperbolic maps are dense. Apparently, up to the late 1960's, Smale believed that hyperbolic systems are dense in all dimensions, but this was shown to be false in the early 1970's for diffeomorphisms on manifolds of dimension ≥ 2 (by Newhouse and others).

Oleg Kozlovski
Mathematics Institute Zeeman Building, University of Warwick, Coventry CV4 7AL, England, UK, e-mail: oleg@maths.warwick.ac.uk

Sebastian van Strien
Mathematics Department, University of Warwick, Coventry CV4 7AL, England, UK, e-mail: strien@maths.warwick.ac.uk

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However, in dimension one hyperbolic systems are dense. This is the topic of this article.

2 Density of Hyperbolicity

The problem of density of hyperbolicity in dimension one goes back in some form to Fatou (in the 1920's). Smale gave this problem 'naively' as a thesis problem in the 1960's (to Guckenheimer and Nitecki), see [12]. The problem whether hyperbolicity is dense in dimension one was studied by many people, and it was solved in the C^1 topology by Jakobson, see [3] and the C^2 topology by Shen [11].

Theorem 1 (K, Shen, vS, 2004). *Any real polynomial can be approximated by hyperbolic real polynomials of the same degree.*

(So by changing the coefficients of the polynomial slightly, it can be made hyperbolic.) Here we say that a real one-dimensional map f is *hyperbolic* if each critical point is in the basin of a (hyperbolic) periodic point and all periodic points are hyperbolic. This implies that the real line is the union of a repelling hyperbolic set (a Cantor set of zero Lebesgue measure), the basin of hyperbolic attracting periodic points and the basin of infinity. So the dynamics of a hyperbolic map is very simple: Lebesgue almost all points are attracted to periodic cycles.

This theorem has a long history before it was proven in this full generality, see works of Yoccoz [14], Sullivan [13], Lyubich [9, 10], Świątek, Graczyk [2], Kozlovski [5], Blokh, Misiurewicz [1], Shen [11]. Most of these works deal with the quadratic family $x \mapsto ax(1-x)$. This case is special, because in this case certain return maps become almost linear. This special behaviour does not even hold for maps of the form $x \mapsto x^4 + c$.

Note that the above theorem implies that the space of hyperbolic polynomials is an open dense subset in the space of real polynomials of fixed degree. Every hyperbolic map satisfying the mild "no-cycle" condition (critical points are not eventually mapped onto other critical points) is structurally stable.

The above theorem allows us to solve the 2nd part of Smale's eleventh problem for the 21st century.

Theorem 2. *Hyperbolic maps are dense in the space of C^k maps of the compact interval or the circle, $k = 1, 2, \ldots, \infty, \omega$.*

As mentioned, this easily implies

Corollary 3. *Structurally stable maps are dense in the space of C^k maps of the compact interval or the circle, $k = 1, 2, \ldots, \infty, \omega$.*

A similar question about density of hyperbolic maps can be asked for maps of a complex plane given by a complex polynomial. In the case of a complex polynomial, we say it is *hyperbolic* if all its critical points are in the basins of hyperbolic periodic attractors. We have only a partial result which applies to non (or finitely) renormalizable polynomials:

Theorem 4. *Any complex polynomial which is not infinitely often renormalizable, can be approximates by a hyperbolic polynomial of the same degree.*

(If we could prove this without the condition that the map is only finitely renormalizable, the complex Fatou conjecture would follows.) Here we say that a polynomial f is *infinitely renormalizable* if there exist arbitrarily large $s > 1$ (called the *period*) and simply connected open sets W containing a critical point c of f such that $f^{ks}(c) \in W, \forall k \geq 0$ and such that s is the first return time of c to W.

3 Quasi-Conformal Rigidity

The proof of these result heavily depends on complex analysis. In fact the theorems above can be derived from the following rigidity result.

Theorem 5. *Let f and $\tilde{f}$ be real polynomials of degree n which only have real critical points. If f and $\tilde{f}$ are topologically conjugate (as dynamical systems acting on the real line) and corresponding critical points have the same order, then they are quasiconformally conjugate (on the complex plane).*

A critical point c is a point so that $f'(c) = 0$. Not all critical points of a real polynomial need to be real.

If the polynomials are not real, then we need to make an additional assumption:

Theorem 6. *Let f and $\tilde{f}$ be complex polynomials of degree n which are not infinitely renormalizable and only have hyperbolic periodic points. If f and $\tilde{f}$ are topologically conjugate, then they are quasiconformally conjugate.*

This generalises the famous theorem of Yoccoz, proving that the Mandelbrot set associated to the quadratic family $z \mapsto z^2 + c$ is locally connected at non-renormalizable parameters.

4 How to Prove Rigidity?

First we need to associate a puzzle partition to any polynomial f which only has hyperbolic periodic points, and then use this to construct a complex box mapping $F\colon U \to V$. If f has only repelling periodic points, then the construction is a multi-critical analogue of the usual Yoccoz puzzle partition.

Definition 7 (Complex box mappings). We say that a holomorphic map

$$F : U \to V \tag{1}$$

between open sets in $\mathbb{C}$ is a *complex box mapping* if the following hold:

- V is a union of finitely many pairwise disjoint Jordan disks;
- Every connected component V' of V is either a connected component of U or the intersection of V' and U is a union of Jordan disks with pairwise disjoint closures which are compactly contained in V',
- For each component U' of U, $F(U')$ is a component of V and $F|U'$ is a proper map with at most one critical point;
- Each connected component of V contains at most one critical point of F.

It is possible to show that for a given polynomial which only has hyperbolic periodic point one can construct an induced complex box mapping which captures the dynamics of the polynomial, see [6].

A connected component of the domain of definition of an iterate of F is called a puzzle-piece. To prove the above rigidity theorem, the main technical hurdle is to obtain a certain amount of control on the shape of these puzzle-pieces. In fact, it is not possible to obtain this control for all puzzle-pieces (and there are examples showing this), however we can prove that this control can be obtained on a combinatorially defined subsequence of puzzle-pieces:

Theorem 8 (Geometry control of puzzle-pieces). *Let F be a complex non renormalizable box mapping and c be a recurrent critical point. Then there exists $\epsilon > 0$ and a combinatorially defined sequence of puzzle-pieces $\mathbf{I}_n$ around c so that*

- *the puzzle-pieces $\mathbf{I}_n$ have ϵ-bounded geometry;*
- *for each domain A of the first return map to $\mathbf{I}_n$ one has* $\mathrm{mod}\,(\mathbf{I}_n \setminus A) \geq \epsilon$.

Here we say that a simply connected domain $U \subset \mathbb{C}$ has ϵ-bounded geometry if there are two disks D_1 and D_2 such that $D_1 \subset U \subset D_2$ and the ratio of diameters of D_1 and D_2 is bounded from below by ϵ.

This control of geometry of puzzle-pieces is enough to prove the Rigidity theorems, because it allows us to apply the following new way of constructing quasiconformal conjugacies:

Theorem 9 (QC-Criterion). *For any constant $\epsilon > 0$ there exists a constant K with the following properties. Let $\phi\colon \Omega \to \tilde{\Omega}$ be a homeomorphism between two Jordan domains. Let X be a subset of Ω consisting of pairwise disjoint topological open discs X_i. Assume moreover,*

1. *For each i both X_i and $\phi(X_i)$ have ϵ-bounded geometry and moreover*

$$mod(\Omega - X_i), mod(\tilde{\Omega} - \phi(X_i)) \geq \epsilon.$$

2. *ϕ is conformal on $\Omega - X_i$.*

Then there exists a K-qc map $\psi\colon \Omega \to \tilde{\Omega}$ which agrees with Ω on the boundary of Ω.

4.1 The Strategy of the Proof of QC-Rigidity

So the proof of the rigidity theorem relies on the following steps:

First we associate to the polynomial f a suitable sequence of partitions $\mathscr{P}_n$. Let Ω_n be a union of puzzle piece containing the critical points, defined using

the puzzle-pieces $\mathbf{I}_n$ from Theorem 8. Because of the geometric properties of $\mathbf{I}_n$, one has control on the domains of the first return map to Ω_n, in the manner required by the previous criterion. This is only true provided one constructs the sequence of partitions $\mathscr{P}_n$ very carefully. Let X_n be the domain of the first return map to Ω_n.

We can do the same for the topologically conjugate polynomial $\tilde{f}$. Now f and $\tilde{f}$ are conformally conjugate near ∞ (by the Böttcher coordinates). Since $\partial\Omega_n$ consists of pieces of external rays and equipotentials, one can show that there exists a qc homeomorphism $\phi_n\colon \Omega_n \to \tilde{\Omega}_n$ (which on the boundary of Ω_n preserves the natural parametrisation induced by the Böttcher coordinates). Moreover, $\phi_n(X_n) = \tilde{X}_n$ and ϕ_n is conformal outside X_n. Hence, because of the control on the geometry of puzzle pieces, the QC-criterion gives a K-qc homeomorphism $h_n\colon \Omega_n \to \tilde{\Omega}_n$ which preserves the natural parametrisation on the boundary defined by the Böttcher coordinates. Here K does not depend on n.

Because $h_n\colon \Omega_n \to \tilde{\Omega}_n$ is natural on the boundary, the above qc map h_n can be extended to a global homeomorphism h_n which is K-qc and so that

$$h_n \circ f(x) = \tilde{f} \circ h_n(x)$$

for each $x \notin \Omega_n$. (So h_n is a conjugacy everywhere except on the small set Ω_n.)

Since K-qc homeomorphisms form a compact space, we can extract a K-qc limit h from the sequence h_n. As Ω_n shrinks to the set of critical points, the limit h is a K-qausi-conformal conjugacy between f and $\tilde{f}$.

5 Enhanced Nest Construction

As we have mentioned before the geometry estimates do not hold for all puzzle-pieces and we have to find a way to combinatorially construct a subsequence of puzzle-pieces where this property holds. This is achieved through a powerful construction which we call "enhanced nest".

For simplicity of the exposition let us consider a unicritical box mapping $F : U \to V$ (*ie* F has a unique critical point) and write $U = \cup U_i$ where U_i are the connected components of the domain U. In this case we can assume that U is a subset of V and V is connected. Let U_0 be a component of U containing the critical point. Consider the critical value $F(c)$ and iterates of F near the critical value. Let us only discuss the case when c is recurrent (the non-recurrent case is much easier). It can happen that there are infinitely many domains W_i containing $F(c)$ and n_i such that F^{n_i} maps W_i univalently onto V for a suitable choice of n_i. This case is called *reluctantly recurrent*. This case is easy: c is recurrent, so there are infinitely many n_{i_j} such that $F^{n_{i_j}+1}(c)$ is inside U_0. The pullback of U_0 by $F^{n_{i_j}+1}$ is a puzzle-piece and then one can easily show (using the Koebe lemma) that its geometry depends only on U_0.

The opposite case, when this infinite sequence of iterates $F^{n_i} : W_i \to V$ does not exist, is called *persistently recurrent*. The enhanced nest construction applies to this case.

If the infinite sequence as above does not exist, then we can consider a minimal domain W around $F(c)$ such that W is univalently mapped onto V by some F^n. This domain W has several nice properties.

Firstly, F^n maps the critical value $F(c)$ into the critical domain U_0. Indeed, otherwise $F^{n+1}(c)$ would be in some domain U_i which is mapped univalently onto V by F; then $F^{n+1} : \mathrm{comp}_{F(c)}(F^{-n}(U_i)) \to V$ is a univalent map which contradicts the minimality of W. Here the notation $\mathrm{comp}_x(U)$ denotes a connected component of U containing x. Secondly, the annulus $W \setminus \tilde{W}$, where $\tilde{W}\mathrm{comp}_{F(c)}(F^{-n}(U_0))$ is a pullback of the central domain, does not contain points of the postcritical set. Suppose the contrary, so there is $k > 0$ such that $F^k(c) \in W \setminus \tilde{W}$ and let k be minimal with this property. Since $F^k(c)$ is not in $\tilde{W}$, the point $F^{k+n}(c)$ is in some non central domain U_j. Let X be a pullback of U_j by F^{k+n-1} along the orbit of the critical value $F(c)$, so $F(c) \in X$. Notice that $F^n : F^{k-1}(X) \to U_j$ is univalent and that $F^{k-1}(X) \subset W \setminus \tilde{W}$. Moreover, $F^{k-1} : X \to F^{k-1}(X)$ is also univalent because of the minimality of k. Hence the map $F^{k+n} : X \to V$ is univalent and this again contradicts the minimality of W.

The pullback of the domain W by $F\colon U \to V$ to the critical point we call the *smallest successor* of V and denoted by $\mathscr{B}(V)$. The corresponding pullback of $\tilde{W}$ will be denoted by $\mathscr{A}(V)$. From the construction the smaller successor we know that $\mathscr{A}(V)$ has some space outside which contains no postcritical points and the $\mathscr{B}(V)$ has some space inside near the boundary free of the postcritical set. Thus, if we combine both operations, we see that $\mathscr{B}(\mathscr{A}(V))$ has some space inside and outside free of the postcritical set. The size (in terms of moduli) of this 'empty' space can be easily estimated if one has estimates from below on $\inf_i \mod (V \setminus U_i)$.

Obviously, this property of having some space around the boundary of a domain free of postcritical set is very important: if $F^m : X \to Y$ is a univalent map between two simply connected domains and $Y' \supset Y$ is another simply connected domain such that the annulus $Y' \setminus Y$ does not contain points of the postcritical set, then there is a domain $X' \supset X$ so that F^m extends to X', $F^m(X') = Y'$ and the map $F^m : X' \to Y'$ is univalent. If one can control the modulus of $Y' \setminus Y$, then the distortion of $F^m|_X$ can be controlled by the classical Koebe lemma.

In the unimodal case we define $\Gamma(W) = \mathscr{B}(W)$. Now, the enhanced nest construction goes as following: given V, let

$$\mathbf{I}_0 := V \text{ and } \mathbf{I}_{i+1} := \Gamma^T(\mathscr{B}(\mathscr{A}(\mathbf{I}_i))),$$

where T only depends on the order of the critical point. We have already explained the rationale behind taking $\mathscr{B}(\mathscr{A}(\mathbf{I}_i))$. The Γ operation is used to control the return times of the critical point to the domains $\mathbf{I}_i$ and is—in some sense—a rather minor technical point.

This is a full description of the enhanced nest in the unicritical case. The construction in the general case is slightly more complicated and then the definitions of $\mathscr{A}(V)$ and $\mathscr{B}(V)$ are based on the following lemma:

Lemma 10. *Let $F : U \to V$ be a persistently recurrent box mapping, c be a critical point of F and $Y \ni c$ be some pullback of a connected component of V by an iterate of F. Then there is a positive integer ν with $F^\nu(c) \in Y$ such that the following holds. Let $X_0 = comp_c(F^{-\nu}(Y))$ and $X_j = F^j(X_0)$ for $0 \le j \le \nu$. Then*

1. $\#\{0 \le j \le \nu - 1 : X_j \cap Crit(F) \neq \emptyset\} \le b^2$;
2. $X_0 \cap PC(F) \subset comp_c(F^{-\nu}(\tilde{Y}))$;

where $Crit(F)$ denotes the set of critical points of F, $PC(F)$ is the postcritical set, b is the number of critical points counted with their multiplicity and $\tilde{Y}$ is a connected component of the domain the first return map to Y containing c.

6 Small Distortion of Thin Annuli

To control the shape of the puzzle-pieces we must control the amount of space around a puzzle-piece which is free of points of the postcritical set. As the previous construction of the enhanced nest shows we should estimate the modulus of pullbacks of various annuli.

Let $G : U \to V$ be a holomorphic surjective map and the domains $A \subset U$, $B \subset V$ be simply connected so that $G(A) = B$. We would like to have some estimates from below of the modulus of the annulus $U \setminus A$ in terms of the modulus of $V \setminus B$. If G is univalent map, this is the best case scenario: mod $(U \setminus A) =$ mod $(V \setminus B)$. Now suppose that G has some critical points and all of them are in A. Then $G : U \setminus A \to V \setminus B$ is an unbranched covering, hence mod $(U \setminus A) =$ mod $(V \setminus B)/d$, where d is the degree of G. If d is large, the modulus can deteriorate quite a lot and one can do nothing about it.

An important case is when G has relatively small number of critical points in A and possibly a large number of critical points in $U \setminus A$. Simple examples show that if the annulus $V \setminus B$ was fat (has large modulus), the modulus of its pullback $U \setminus A$ can drop a lot. However there is a special case when this does not happen: if the annulus $V \setminus B$ is thin, the map G is real and all the domains are symmetric with respect to the real line. More precisely the following lemma holds:

Lemma 11 (Small Distortion of Thin Annuli). *For every $K \in (0, 1)$ there exists $\kappa > 0$ such that if $A \subset U$, $B \subset V$ are simply connected domains symmetric with respect to the real line, $G : U \to V$ is a real holomorphic branched covering map of degree D with all critical points real which can be decomposed as a composition of maps $G = g_1 \circ \cdots \circ g_n$ with all maps g_i real and either real univalent or real branched covering maps with just one critical point, the domain A is a connected component of $G^{-1}(B)$ symmetric with respect to the real line and the degree of $G|_A$ is d, then*

$$\mathrm{mod}\ (U \setminus A) \geq \frac{K^D}{2d} \min\{\kappa, \mathrm{mod}\ (V \setminus B)\}.$$

It is not possible to drop the condition of G being real and the domains being symmetric. If V is a disk and B spirals around its centre (and therefore not symmetric with respect to the real line), it is possible to construct G so that the lemma does not hold.

This lemma allowed us to considerably simplify the original proof of the real Geometry control of puzzle-pieces theorem (which initially used many sophisticated real pullback arguments). The basic idea how to use the lemma in order to prove Theorem 8 is this: let $\mu_n = \inf \mathrm{mod}(\mathbf{I}_n \setminus A)$ where the infimum runs over all domains A of the first return map to $\mathbf{I}_n$. Now consider the iterate G of F which maps $\mathbf{I}_n$ to $\mathbf{I}_{n-M}$. When M is large, the degree D of this map is large. However, it turns out that

- the degree d of $G|_A$ remains bounded, independently of M;
- the set $\mathbf{I}_{n-M} \setminus G(A)$ contains many 'previous annuli', and using this we get: $\mathrm{mod}\ (\mathbf{I}_{n-M} \setminus G(A)) \geq K'(\mu_{n-M-1} + \cdots + \mu_{n-5})$, where K' is independent of M.

Now fix M so large that $K'(\mu_{n-M-1} + \cdots + \mu_{n-5}) \geq 8d\mu_{n-M-1,n-5}$ where $\mu_{n-M-1,n-5} = \min\{\mu_i;\ i = n - M - 1, \ldots, n - 5\}$. Next choose $K \in (0, 1)$ so close that $K^D \geq 1/2$. Using the previous lemma we then get some $\kappa > 0$ so that $\mathrm{mod}\ (\mathbf{I}_n \setminus A) \geq \frac{1/2}{2d} \min(\kappa, 8d\ \mu_{n-M-1,n-5})$. From this one easily proves recursively a lower bound for μ_n. The proof of Theorem 8 follow then easily.

The proof of the previous lemma is relatively simple and is based on the following idea. We can cut B into two symmetrical pieces by the real line and pullback just a half of B by maps g_i. All the pullbacks are going to lay in a half complex plain, and it is possible to provide good moduli estimates for this case. When the half of B is pullbacked all the way to U we can reconstruct A from it by the symmetry. In this last operation we loose only factor of one half.

If G is not real, the situation is more complicated because as we mentioned there is not (and cannot be) an analogue of the previous lemma. However, it is still possible to control moduli if one pullbacks two annuli instead of one. The following powerful lemma is due to Kahn and Lyubich, see [4]:

Lemma 12. *For any $\eta > 0$ and $D > 0$ there is $\epsilon = \epsilon(\eta, D) > 0$ such that the following holds: Let $A \subset A' \subset U$ and $B \subset B' \subset V$ be topological disks in $\mathbb{C}$ and let $G : (A, A', U) \to (B, B', V)$ be a holomorphic branched covering map. Let the degree of G be bounded by D and the degree of $G|_{A'}$ be bounded by d. Then*

$$\mathrm{mod}\ (U \setminus A) > \min(\epsilon,\ \eta^{-1}\ \mathrm{mod}\ (B' \setminus B),\ C\eta d^{-2}\ \mathrm{mod}\ (V \setminus B)),$$

where $C > 0$ is some universal constant.

7 Approximating Non-renormalizable Complex Polynomials

If the complex Rigidity theorem were proven in full generality, then using the standard Sullivan technique one could show that the hyperbolic polynomials are dense in the space of complex polynomials of fixed degree. We have proven the complex Rigidity theorem in the case of finitely renormalizable polynomials, so some extra work is needed to show that such polynomials can be approximated by hyperbolic ones.

To simplify the exposition we will show how to do this in the case of cubic non renormalizable polynomial whose both critical points are recurrent. We can normalise a cubic polynomial so it is $f(z) = z^3 + az + b$.

The Rigidity theorem implies that there are no other normalised polynomials qc conjugate to f. Fix some neighbourhood W of f in the space of cubic normalised polynomials. For $g \in W$ let $c_k(g)$, $k = 1, 2$, denote the critical points of g.

First we claim that there are polynomials in W which have a critical relation, i.e. there are k_1, k_2, n such that $g^n(c_{k_1}(g)) = c_{k_2}(g)$. Indeed, if this was not the case, all preimages of the critical points would move holomorphically as functions of $g \in W$. Then using Lambda lemma we can extend this holomorphic motion to the whole $\mathbb{C}$ and get that all polynomials in W are qc conjugate.

The neighbourhood W can be chosen arbitrarily small, and therefore there are polynomials arbitrarily close to f having a critical relation. Any critical relation gives an algebraic curve in the space of normalised cubic polynomials (which is $\mathbb{C}^2$), this curve contains all polynomials having the same critical relation.

Consider one of these curves. Since it is an algebraic curve it has just finitely many singular points, we can remove them from this curve and get a holomorphic one dimensional manifold. Take some connected component of the intersection of W and this manifold which will be denoted by M_1 and take a polynomial $f_1 \in M_1$. Arguing as before we can see that either all polynomials in M_1 are qc conjugate or there is polynomial in M_1 having another critical relation. If a cubic polynomial has two critical relations, then it is hyperbolic. So if the second alternative holds, we are done because we have found a hyperbolic polynomial in W. If all polynomials in M_1 are qc conjugate, we cannot apply the Rigidity theorem because we do not know whether f_1 is finitely renormalizable or not. Instead we should do the following.

Take a sequence of polynomials f_i having a critical relations and converging to f. Let $M_i \ni f_i$ denote connected components of intersection of W and the corresponding manifolds as in the previous paragraph. We can assume that all polynomials in M_i are qc conjugate (otherwise we are done). The closure of each M_i has non empty intersection with the boundary of W because M_i is a part of an algebraic curve and such curves cannot have compact components in $\mathbb{C}^2$. Therefore we can find $\tilde{f} \in \partial W$, a subsequence i_j and $\tilde{f}_{i_j} \in M_{i_j}$ so that $\tilde{f}_{i_j}$ converges to $\tilde{f}$. The maps f_{i_j} and $\tilde{f}_{i_j}$ are qc conjugate and $f_{i_j} \to f$, so it is possible to show (though it is not completely straightforward) that the maps f and $\tilde{f}$ are qc conjugate as well. Now we can apply the Rigidity theorem because f is non renormalizable and we can see that such the polynomial $\tilde{f}$ cannot exist.

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Large Gap Asymptotics for Random Matrices

Igor Krasovsky

Abstract Asymptotic behavior is discussed of the sine-kernel and Airy-kernel Fredholm determinants related to random matrices.

Let $K_s^{(j)}$, $j = 1, 2$ be the trace-class operators with kernels

$$K_s^{(1)}(x, y) = \frac{\sin(x - y)}{\pi(x - y)}, \qquad K_s^{(2)}(x, y) = \frac{\mathrm{Ai}(x)\mathrm{Ai}'(y) - \mathrm{Ai}(y)\mathrm{Ai}'(x)}{x - y} \tag{1}$$

acting on $L^2(0, 2s)$ and $L^2(-s, \infty)$, respectively. We are interested in the behaviour of the following Fredholm determinants, the so called sine-kernel and Airy-kernel determinants,

$$P_s^{(j)} = \det(I - K_s^{(j)}), \quad j = 1, 2, \tag{2}$$

as $s \to +\infty$. In the Gaussian Unitary Ensemble of random matrices [11], $P_s^{(1)}$ is the probability, in the bulk scaling limit, that there are no eigenvalues in the interval $(0, 2s)$; while $P_s^{(2)}$ is the probability, in the edge scaling limit, that there are no eigenvalues in the interval $(-s, +\infty)$ ($P_s^{(2)}$ is the distribution of the largest eigenvalue). The asymptotics of $P_s^{(j)}$ as $s \to +\infty$ are often referred to as the large gap asymptotics.

We will describe the main steps of the method of computing the asymptotics of $P_s^{(j)}$ used in [4, 5, 10]. However, we leave out all the Riemann-Hilbert analysis and just state its results when needed. The details are given in the 3 mentioned publications.

First, we discuss the case of the sine-kernel. In [7], Dyson found that

Igor Krasovsky
Department of Mathematical Sciences, Brunel University West London, Uxbridge UB83PH, UK, e-mail: Igor.Krasovsky@brunel.ac.uk

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$$\ln P_s^{(1)} = -\frac{s^2}{2} - \frac{1}{4}\ln s + c_0 + \frac{a_1}{s} + \frac{a_2}{s^2} + \cdots, \quad s \to +\infty, \tag{3}$$

where

$$c_0 = \frac{1}{12}\ln 2 + 3\zeta'(-1). \tag{4}$$

Here $\zeta(z)$ is the Riemann zeta-function. The constants a_1, a_2, were also identified in [7]. The first 2 leading terms in the expansion (3) were found earlier by des Cloizeaux and Mehta [6]. The results in [6] and [7] were not fully rigorous.

The fact that the first leading term in (3) is correct was proved in [14] by Widom. The full asymptotic expansion of $(d/ds)\ln P_s$ was obtained rigorously by Deift, Its, and Zhou in [3]. This result proves (3) up to the expression for c_0. The final step, a proof that c_0 is given by (4), was carried out recently and in 3 variants: by Ehrhardt [8], by the author [10], and by Deift, Its, Zhou, and the author in [4]. The methods of [10] and [4] are closely related and we will now describe a "hybrid" approach based on these 2 papers.

For a function $f(\theta)$ integrable over the unit circle, the Toeplitz determinant with symbol f is given by the expression:

$$D_n(f) = \det\left(\frac{1}{2\pi}\int_0^{2\pi} e^{-i(j-k)\theta} f(\theta)d\theta\right)_{j,k=0}^{n-1}. \tag{5}$$

A Toeplitz determinant has the following two useful representations:

$$D_n(f) = \frac{1}{(2\pi)^n n!}\int_0^{2\pi}\cdots\int_0^{2\pi}\prod_{1\le j<k\le n}|e^{i\theta_j} - e^{i\theta_k}|^2\prod_{j=1}^{n} f(\theta_j)d\theta_j, \tag{6}$$

and

$$D_n(f) = \prod_{j=0}^{n-1}\chi_k^{-2}, \tag{7}$$

where χ_k are the leading coefficients of the polynomials $\phi_k(z) = \chi_k z^k + \cdots$, $k = 0, 1, \ldots$ orthogonal with weight $f(\theta)$ on the unit circle. If $f(\theta)$ is real and nonnegative,

$$\frac{1}{2\pi}\int_0^{2\pi}\phi_k(e^{i\theta})\overline{\phi_m(e^{i\theta})}f(\theta)d\theta = \delta_{km}, \quad k, m = 0, 1, \ldots. \tag{8}$$

To obtain the asymptotics of the Fredholm determinants, we represent them as double-scaling limits of Toeplitz (for the sine-kernel case) and Hankel (for the Airy-kernel case, see below) determinants. Let

$$f(\theta) \equiv f_\alpha(\theta) = \begin{cases} 1, & \alpha < \theta < 2\pi - \alpha \\ 0, & \text{otherwise.} \end{cases} \tag{9}$$

Now observe that

$$P_s^{(1)} = \lim_{n\to\infty} D_n(f_{2s/n}). \tag{10}$$

This fact is actually used in random matrix theory to obtain the sine-kernel determinant; it was also used by Dyson in [7]. Note that if we could find the asymptotics of the polynomials orthogonal with weight (9), and in particular, the asymptotics of χ_k, $k \to \infty$, we would obtain by (10) and (7) part of (3) but not the constant c_0, as the product of the first $\chi_0\chi_1\cdots\chi_{k_0}$ would remain undetermined. However, this difficulty can be resolved. We start with the following identity, which can be obtained from (7):

$$\frac{d}{d\alpha}\ln D_n(f_\alpha) = \frac{n}{\pi}|\phi_n(e^{i\alpha},\alpha)|^2 - \frac{1}{\pi}\left\{\phi_n(e^{-i\alpha},\alpha)e^{i\alpha}\phi_n'(e^{i\alpha},\alpha) + \text{c.c.}\right\},$$
$$n = 1, 2, \ldots \tag{11}$$

where $\phi_k(z,\alpha)$ are the polynomials orthogonal w.r.t. f_α given by (9), and $\phi_k'(z,\alpha)$ are their derivatives w.r.t. the variable z. To use this identity, we now need to find the asymptotics of the polynomials appearing in the r.h.s. We do this by solving the Riemann-Hilbert problem associated with these polynomials using a steepest descent approach of Deift and Zhou [2]. (Riemann-Hilbert formulation for orthogonal polynomials was first observed in the case of orthogonality on the real line by Fokas, Its, and Kitaev in [9].) This step of the analysis is technically the most involved one. If we substitute the results in the r.h.s. of (11), we obtain

$$\frac{d}{d\alpha}\ln D_n(f_\alpha) = -\frac{n^2}{2}\tan\frac{\alpha}{2} - \frac{1}{8}\cot\frac{\alpha}{2} + O\left(\frac{1}{n\sin^2(\alpha/2)}\right) \tag{12}$$

for all $n > s_0$ with some fixed s_0. A crucial fact is that this expansion holds and the error term is uniform for $\frac{2s_0}{n} \le \alpha < \pi$. We will now integrate this identity.

First, we can obtain an expression for $D_n(f_\alpha)$ as $\alpha \to \pi$ from below. Changing the variables $\theta_j = \pi + (\pi-\alpha)x_j$ in (6) and expanding the integrand in $\pi - \alpha$, we obtain

$$D_n(f_\alpha) = \frac{1}{(2\pi)^n n!}\int_\alpha^{2\pi-\alpha}\cdots\int_\alpha^{2\pi-\alpha}\prod_{1\le j<k\le n}|e^{i\theta_j} - e^{i\theta_k}|^2\prod_{j=1}^n d\theta_j$$
$$= \frac{(\pi-\alpha)^{n^2}}{(2\pi)^n}A_n(1 + O_n((\pi-\alpha)^2)), \tag{13}$$

as $\alpha \to \pi$ from below and n is fixed. Here

$$A_n = \frac{1}{n!}\int_{-1}^1\cdots\int_{-1}^1\prod_{1\le j<k\le n}(x_j - x_k)^2\prod_{j=1}^n dx_j = 2^{n^2}\prod_{k=0}^{n-1}\frac{k!^3}{(n+k)!} \tag{14}$$

is a Selberg integral. Using its asymptotics as $n \to \infty$, we obtain from (13)

$$\ln D_n(f_\alpha) = n^2 \ln \frac{\pi - \alpha}{2} - \frac{1}{4} \ln n + c_0 + \delta_n + O_n((\pi - \alpha)^2), \quad \alpha \to \pi, \quad (15)$$

where c_0 is given by (4) and $\delta_n \to 0$ as $n \to \infty$ (δ_n depends only on n).

Now we can integrate the identity (12) from α close to π to $\alpha \geq 2s_0/n$ and use (15) at the lower integration limit. We thus obtain the following general formula:

$$\ln D_n(\alpha) = n^2 \ln \cos \frac{\alpha}{2} - \frac{1}{4} \ln\left(n \sin \frac{\alpha}{2}\right) + c_0 + O\left(\frac{1}{n \sin(\alpha/2)}\right) + \delta_n, \quad (16)$$

for $\frac{2s_0}{n} \leq \alpha < \pi$, $n > s_0$, where s_0 is a (large) positive constant.

Note that for a fixed α, as $n \to \infty$ (16) reproduces a result of Widom [13] for the asymptotics of a determinant on a fixed arc of the unit circle, which was used by Dyson to conjecture the value of c_0 (4).

Setting $\alpha = 2s/n$, $s > s_0$ in (16), and letting $n \to \infty$, we obtain by (10)

$$P_s^{(1)} = \lim_{n\to\infty} D_n(f_{2s/n}) = -\frac{s^2}{2} - \frac{1}{4} \ln s + c_0 + O\left(\frac{1}{s}\right), \quad (17)$$

with c_0 given by (4). This, in particular, completes the proof for the constant term c_0 in (3). Note that the present approach can be used to compute further terms in the asymptotic expansion.

We now turn our attention to the Airy-kernel determinant, $P_s^{(2)}$, known as the Tracy-Widom distribution. In [12], Tracy and Widom found a connection of $P_s^{(2)}$ with the Hastings-McLeod solution of the Painlevé II equation, and also observed that

$$\ln \det(I - K_s) = -\frac{s^3}{12} - \frac{1}{8} \ln s + \chi + \frac{b_3}{s^3} + \frac{b_6}{s^6} + \cdots, \quad \text{as } s \to +\infty, \quad (18)$$

where the values of $b_3, b_6, \ldots$ are extracted from the asymptotics of the Hastings-McLeod solution, and

$$\chi = \frac{1}{24} \ln 2 + \zeta'(-1). \quad (19)$$

This value of χ was conjectured in [12] based on numerical evidence and by taking into account a similar expression for the constant c_0 in (4). A proof was given by Deift, Its, and the author in [5], and another proof by Baik, Buckingham, and DiFranco appeared in [1]. Here we discuss the approach used in [5], stressing its similarities to the method in the case of the sine-kernel described above.

For a function $w(x)$ integrable over the real half-line $(0, \infty)$, consider the Hankel determinant with symbol w:

$$D_n^H(w) = \det\left(\int_0^\infty x^{j+k} w(x) dx\right)_{j,k=0}^{n-1}. \quad (20)$$

Just as in the case of a Toeplitz determinant, the Hankel determinant D_n^H has the following two useful representations:

$$D_n^H(w) = \frac{1}{n!}\int_0^\infty \cdots \int_0^\infty \prod_{1\le j<k\le n}(x_j - x_k)^2 \prod_{j=1}^n w(x_j)dx_j, \tag{21}$$

and

$$D_n^H(w) = \prod_{j=0}^{n-1} \varkappa_k^{-2}, \tag{22}$$

where $\varkappa_k$ are the leading coefficients of the polynomials $p_k(x) = \varkappa_k x^k + \cdots$, $k = 0, 1, \ldots$ orthogonal with weight $w(x)$ on the real half-line. If $w(x)$ is real and nonnegative,

$$\int_0^\infty p_k(x)p_m(x)w(x)dx = \delta_{km}, \quad k, m = 0, 1, \ldots. \tag{23}$$

Let

$$w(x) \equiv w_\alpha(x) = \begin{cases} e^{-4xn}, & 0 < x < \alpha \\ 0, & \text{otherwise.} \end{cases} \tag{24}$$

With so defined $w_\alpha(x)$, the following analogue of (10) holds:

$$P_s^{(2)} = \lim_{n\to\infty} \frac{D_n^H(w_{1-s/(2n)^{2/3}})}{D_n^H(w_\infty)}. \tag{25}$$

Using (22) we can obtain the following differential identity:

$$\frac{d}{d\alpha}\ln D_n^H(w_\alpha) = \frac{\varkappa_{n-1}(\alpha)}{\varkappa_n(\alpha)} e^{-4n\alpha}(p_n'(\alpha,\alpha)p_{n-1}(\alpha,\alpha) - p_n(\alpha,\alpha)p_{n-1}'(\alpha,\alpha)), \tag{26}$$

where $p_k(x,\alpha) = \varkappa_k(\alpha)x^k + \cdots$ are the polynomials orthogonal on $(0,\alpha)$ with weight $w_\alpha(x)$, and the prime denotes differentiation w.r.t. the argument x.

A Riemann-Hilbert analysis of the polynomials $p_k(x,\alpha)$ as $k \to \infty$ produces the asymptotic expression for the r.h.s. of (26), and we have

$$\frac{d}{d\alpha}\ln D_n^H(w_\alpha) = \frac{n^2}{\alpha}(1-\alpha)^2 + \frac{\alpha}{4(1-\alpha^2)} + \frac{1}{1-\alpha}O\left(\frac{1}{n|1-\alpha|^{3/2}}\right). \tag{27}$$

This expansion holds uniformly in $\alpha \in (0, 1 - s_0/(2n)^{2/3}]$ for all $n > s_0^{3/2}/2$, where s_0 is some (large) fixed number.

To proceed as in the case of the sine-kernel, we estimate first $D_n^H(w_\alpha)$ for $\alpha \to 0$, where a series expansion can be written. This is done by an analysis of (21), and we obtain (cf. the derivation of (13)):

$$D_n^H(w_\alpha) = \frac{1}{n!}\int_0^\alpha \cdots \int_0^\alpha \prod_{0\le i<j\le n-1}(x_i - x_j)^2 \prod_{j=0}^{n-1} e^{-4x_j n} dx_j$$
$$= \left(\frac{\alpha}{2}\right)^{n^2} A_n(1 + O_n(\alpha)), \tag{28}$$

as $\alpha \to 0$ from above and n is fixed. The quantity A_n is a Selberg integral given by (14). Note that $D_n^H(w_\infty)$ is another Selberg integral:

$$D_n^H(w_\infty) = \frac{1}{n!}\int_0^\infty \cdots \int_0^\infty \prod_{0\le i<j\le n-1}(x_i - x_j)^2 \prod_{j=0}^{n-1} e^{-4x_j n} dx_j$$
$$= (4n)^{-n^2} \prod_{k=0}^{n-1} k!^2. \tag{29}$$

(Both A_n and $D_n^H(w_\infty)$ can also be computed using the formula (22) for the Legendre and Laguerre orthogonal polynomials, respectively.)

Using the asymptotics of A_n and $D_n^H(w_\infty)$ for $n \to \infty$, we conclude that (cf. (15))

$$\ln \frac{D_n^H(w_\alpha)}{D_n^H(w_\infty)} = \left(\frac{3}{2} + \ln\alpha\right) n^2 - \frac{1}{12}\ln\frac{n}{2} + \zeta'(-1) + \widetilde{\delta}_n + O_n(\alpha), \quad \alpha \to 0, \tag{30}$$

where $\widetilde{\delta}_n$ depends on n only, and $\widetilde{\delta}_n \to 0$ as $n \to \infty$.

Now we can integrate the identity (27) from α close to 0 to $\alpha \le 1 - s_0/(2n)^{2/3}$ and use (30) at the lower integration limit. We obtain for any $0 < \alpha \le 1 - s_0/(2n)^{2/3}$, and any $n > s_0^{3/2}/2$ (cf. (16)):

$$\ln \frac{D_n^H(w_\alpha)}{D_n^H(w_\infty)} = n^2\left(\frac{3}{2} + \ln\alpha - 2\alpha + \frac{\alpha^2}{2}\right) - \frac{1}{12}\ln n - \frac{1}{8}\ln(1-\alpha^2)$$
$$+ \frac{1}{12}\ln 2 + \zeta'(-1) + O\left(\frac{1}{n(1-\alpha)^{3/2}}\right) + \widetilde{\delta}_n. \tag{31}$$

Set here $\alpha = 1 - s/(2n)^{2/3}$, $s > s_0$, and let $n \to \infty$. By (25) we obtain

$$P_s^{(2)} = \lim_{n\to\infty} \frac{D_n^H(w_{1-s/(2n)^{2/3}})}{D_n^H(w_\infty)}$$
$$= -\frac{s^3}{12} - \frac{1}{8}\ln s + \frac{1}{24}\ln 2 + \zeta'(-1) + O(s^{-3/2}), \tag{32}$$

which gives the first 3 terms of (18). Further terms can be obtained in this way as well.

Let us again stress that our approach [10, 4, 5] to compute the asymptotics for the above Fredholm determinants is based on approximating them with Toeplitz

and Hankel determinants. We then analyse the related systems of orthogonal polynomials, and use identities for the logarithmic derivatives of Toeplitz and Hankel determinants. As a byproduct of this approach, we obtain the asymptotics for the orthogonal polynomials (for weights f_α and w_α).

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On the Derivation of Fourier's Law

Antti Kupiainen*

Abstract We discuss derivation of Fourier's law of heat conduction from a microscopic Hamiltonian dynamics. The model consists of weakly coupled anharmonic oscillators arranged on a three dimensional lattice and subjected to a stochastic forcing on the boundary. We introduce a truncation of the system of equations satisfied by correlation functions of the stationary state of the system which leads to a nonlinear generalized Boltzman equation for the two-point stationary correlation functions. These equations have a unique solution which, for N large, is approximately a local equilibrium state satisfying Fourier law that relates the heat current to a local temperature gradient. The temperature exhibits a nonlinear profile.

1 Introduction

Out of equilibrium systems are ubiquitous in nature. There is a long history of studying them from non-equilibrium statistical mechanics to dynamical systems theory. However, it is fair to say that our mathematical understanding of such phenomena is still in its infancy. I will discuss below attempts to derive Fourier's law in a Hamiltonian extended dynamical system. Stated very briefly, the issue is the following.

If we heat a piece of solid locally and then leave it cool, the initial temperature distribution will diffusively relax to a constant temperature. The process is accompanied by a heat flow that is proportional to the local temperature gradient, according to Fourier's law. Similarly, if we keep on the source of heat a steady state will develop with a temperature distribution across the body accompanied with a steady flow of heat. A mathematical understanding of these phenomena starting from a microscopic model of matter is a considerable challenge [1].

Antti Kupiainen
Department of Mathematics, Helsinki University, P.O. Box 4, 00014 Helsinki, Finland, e-mail: ajkupiai@mappi.helsinki.fi

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This classical problem has received a lot of attention during recent years from mathematical, theoretical and numerical points of view (for some reviews see [8, 10]). To isolate heat transport from other transport processes like particle transport it is convenient to discuss models of solids i.e. models of lattice vibrations where the dynamical variables are attached to points of a d-dimensional lattice. The dynamics consists of two parts: on-site dynamics involving only variables at a given lattice site and interactions or coupling between sites. In general terms two kinds of models have been considered. In the first class dynamics is weakly nonlinear and interactions between sites are order unity. The mechanism behind dissipation lies in the loss of coherence of harmonic waves due to scattering induced by nonlinearity. In the second class of models [5, 4] the on-site dynamics is taken strongly chaotic while perturbation parameter is the interaction between sites. The non-interacting model has a conserved quantity (energy) at each lattice site and interactions lift this degeneracy resulting in a diffusion of the local energies.

We will discuss below the issues related to the derivation of transport in the first class of models: the problem of closure of the equations for correlation functions and the nature of a weak anharmonicity scaling limit and the Boltzmann equation describing it. The second class of models deserve a thorough look in the future, because the actual mathematical proof of Fourier's law is likely to be more accessible there.

2 Coupled Oscillators

A physical theory of heat conduction should start from quantum mechanics, but since we are after macroscopic laws the problem can be posed also classically (which is also physically adequate except in low temperatures). A simple classical mechanical system modeling heat transport in solids is given by a system of coupled oscillators organized on a d-dimensional cubic lattice $\mathbb{Z}^d$. The oscillators are indexed by lattice points $x \in \mathbb{Z}^d$, and carry momenta and coordinates (p_x, q_x). In the simplest model p_x and q_x take real values and their dynamics is generated by a Hamiltonian

$$H(q, p) = \frac{1}{2m} \sum_x p_x^2 + \sum_{xy} U(q_x - q_y) + \sum_x V(q_x), \tag{1}$$

where the second sum is over nearest neighbors. The potential energy U gives rise to interactions (or coupling) between the oscillators and V is the "pinning potential" tying the oscillators to the lattice sites. m is the mass parameter of the oscillator which can be taken to 1 for simplicity.

The problem of transport can be posed in two ways. The first is to consider pure Hamiltonian dynamics

$$\dot{q}_x = p_x \tag{2}$$

$$\dot{p}_x = -\frac{\partial H}{\partial q_x} \tag{3}$$

for an infinite system, the whole $\mathbb{Z}^d$. The dynamics (3) preserves the Gibbs measures in the phase space, formally given by

$$Z^{-1} e^{-\beta H(q,p)} dq\, dp \tag{4}$$

and describing an equilibrium state with constant inverse temperature $\beta = 1/T$. One expects initial states that agree with (4) "at infinity" to be attracted by (4) under the flow (2) (since one works here in infinite volume, one does not expect Poincaré's recurrences to occur). Moreover, the measure should in long times be close to a local equilibrium state parametrized by a spatially and temporally varying temperature and a current tied to the former by Fourier's law while the temperature follows a nonlinear heat equation (see below).

The second approach is to consider a non equilibrium stationary state. Then the system is confined to a subset $V \subset \mathbb{Z}^d$ and one subjects it to a "heat bath" on the boundary ∂V. One way to model this is to add to the force on the RHS of (3) a stochastic force

$$-\gamma p_x + \sqrt{2\gamma T_x}\dot{\beta}_x$$

for $x \in \partial V$ where β_x are independent unit Brownian motions and $T_x > 0$ is the temperature of the heat bath modeled by the noise at the boundary point x. Equations (2) and (3) become then a system of stochastic differential equations and as a consequence the solution $(q(t), p(t))$ is a Markov process instead of a deterministic flow.

The non equilibrium stationary state we are after is a stationary state of this Markov process and one would like to prove its existence and uniqueness as well as properties such as the possible Fourier's law. To state the latter precisely we need to define the temperature distribution and heat flux in V associated to such a stationary state. The former can be defined as the average

$$T_x = E\ p_x^2$$

and the latter by

$$J_x^\mu = -\frac{1}{2} E(p_{x+\mu} + p_x) U'(q_{x+\mu} - q_x)$$

where the expectation is taken in the stationary state and μ is a unit vector.

Both in the dynamic and in the stationary approach to our problem Fourier's law should become an exact statement only in the *scaling limit*. In the stationary approach fix a region Ω in $\mathbb{R}^d$ and let V consist of lattice points in $N\Omega$. Then, letting $\mathscr{T}(x) = T_{Nx}$ and (in the case of normal conductivity) $\mathscr{J}(x) = NJ_{Nx}$, as $N \to \infty$ these should converge to functions satisfying

$$\mathscr{J}(x) = -\kappa(\mathscr{T}(x))\nabla\mathscr{T}(x) \tag{5}$$

$$\nabla \cdot \kappa(\mathscr{T})\nabla\mathscr{T} = 0 \tag{6}$$

where the conductivity κ depends on the local temperature. The latter is a solution of a non linear elliptic equation on Ω with boundary condition on $\partial\Omega$ fixed by the temperature distribution of the heat bath (i.e. amplitude of the noise).

In the dynamical approach one takes an initial measure that is slowly varying in space in the scale N. Then after an appropriate rescaling of space and time one should obtain a parabolic version of (7)

$$\partial_t T = \nabla \cdot \kappa(\mathscr{T})\nabla\mathscr{T} \tag{7}$$

together with the Fourier's law (5) for the current.

3 Closure Equations

Let us consider the Markov process described in the previous section. To fix ideas, let the coupling potential be harmonic, $U(q) = \frac{1}{2}q^2$ and the "pinning" potential be weakly anharmonic,

$$V(q) = \frac{r}{2}q^2 + \lambda q^4$$

with λ small. When $\lambda = 0$ the equilibrium Gibbs measure (4) is a Gaussian measure with inverse covariance

$$\beta(-\Delta + r) := \beta\omega^2 \tag{8}$$

where Δ is the lattice Laplacean. When λ is small this measure is close to Gaussian. It is then not unreasonable to expect that the non equilibrium stationary state is close to Gaussian or that the Markov process when started with a Gaussian state close to the equilibrium state keeps it close to Gaussian all times. An attempt to find a Gaussian approximation for the true stationary state was done in [2] which we will now describe.

We start by deriving equations for the correlation functions of the Markov process $(q(t), p(t))$. Let us denote (q_x, p_x) by (u_{1x}, u_{2x}) and the nonlinear term in (3) by $\Lambda(u)$ i.e. $\Lambda(u)_{\alpha x} = -\lambda\delta_{\alpha,2}q_x^3$. The equation also involves the friction term $(\Gamma u)_x = (0, \gamma_x p_x)$ with $\gamma_x = \gamma$ for $x \in \partial V$ and the noise $\eta = \sqrt{2\gamma T_x}(0, \beta)$. Then the stochastic process $u(t)$ satisfies

$$du(t) = \big((A - \Gamma)u + \Lambda(u)\big)dt + d\eta(t) \tag{9}$$

where $A = \left(\begin{smallmatrix} 0 & 1 \\ -\omega^2 & 0 \end{smallmatrix}\right)$. By an application of the Ito formula the correlation functions

$$G_n(t, x_1, \ldots, x_n) = \langle u_{x_1}(t) \otimes \cdots \otimes u_{x_n}(t)\rangle \in \mathbf{R}^{2nV}$$

satisfy the Hopf equations

$$\dot{G}_N = (A_n - \Gamma_n)G_n + \Lambda_n G_{n+2} + \mathscr{C}_n G_{n-2}. \tag{10}$$

where $A_n = \sum A_{x_i}$ and Γ_n is defined similarly. Λ_n and $\mathscr{C}_n$ are linear operators from $\mathbf{R}^{2(n+2)V} \to \mathbf{R}^{2nV}$ and $\mathbf{R}^{2(n-2)V} \to \mathbf{R}^{2nV}$ respectively involving the trilinear operator Λ and the noise covariance C_{xy} of (8).

The correlation functions in the stationary state of the Markov process should then satisfy the stationary version of (10):

$$(A_n - \Gamma_n)G_n + \Lambda_n G_{n+2} + \mathscr{C}_n G_{n-2} = 0. \tag{11}$$

These equations have the drawback that they do not "close": to solve for G_n, we need to know G_{n+2}. We will now introduce an approximation that will lead to a closed set of nonlinear equations for G_2.

The first equation in the hierarchy (10) reads:

$$(A_2 - \Gamma_2 + \Sigma_2)G_2 + \Lambda_2 G_4^c + \mathscr{C} = 0 \tag{12}$$

where $\Sigma_2(G_2)G_2 = \Lambda_2 \sum G_2 \otimes G_2$ and we introduced G_4^c, the connected correlation function describing deviation from Gaussianity.

For λ small we expect the stationary measure to be close to a Gaussian measure for which G_4^c vanishes. Hence one might look for a Gaussian approximation to the stationary measure by *closing* (12), i.e. ignoring the G_4^c term. This leads to a nonlinear equation for G_2. It turns out that the solution to this equation is qualitatively similar to the $\lambda = 0$ case. In particular G_2 does not exhibit a temperature profile nor a finite conductivity. The only effect of the nonlinearity is a renormalization of ω.

The next equation in the hierarchy becomes after some algebra

$$(A_4 - \Gamma_4 + \Sigma_4)G_4^c + b(G_2) + \Lambda_4 G_6^c = 0, \tag{13}$$

where G_6^c is the connected six point function,

$$\Sigma_4(G_2)G_4^c = \sum (\Lambda_4(G_2 \otimes G_4^c) - G_2 \otimes \Lambda_2 G_4^c),$$

and

$$b(G_2) = \sum_p \Lambda_4'(G_2 \otimes G_2 \otimes G_2),$$

where Λ_4' has Λ acting on all the three factors G_2.

Equations (12) and (13) yield an exact equation for the two point function with the connected six point function as an input. Our closure approximation consists of dropping the G_6^c term in (13) thereby yielding a closed set of equations for G_2. For simplicity we also drop the operators Σ_2, Σ_4 and Γ_4: these could be included in our analysis, but do not change the main structure that is due to the term $b(G_2)$. Hence the closure equation we study is for $G = G_2$:

$$(A_2 - \Gamma_2)G + \mathscr{N}(G) + \mathscr{C} = 0 \tag{14}$$

with

$$\mathscr{N} = -\Lambda_2 A_4^{-1} b(G). \tag{15}$$

To write this more concretely, let us introduce the matrices

$$Q_{xy} = \langle q_x q_y \rangle, \quad P_{xy} = \langle p_x p_y \rangle, \quad J_{xy} = \langle q_x p_y \rangle.$$

Clearly

$$\dot{Q} = J + J^T$$

so the (1, 1)-component of (14) says

$$J_{xy} = -J_{yx}$$

and we can write

$$G = \begin{pmatrix} Q & J \\ -J & P \end{pmatrix}.$$

To proceed let us choose a special geometry by taking the lattice subset V a semi-infinite slab of width N i.e. $V = [0, N] \times \mathbb{Z}^{d-1}$. Next, anticipating translation invariance in the directions orthogonal to the 1-direction we write

$$G(x, y) = \int e^{ip(x_1+y_1)+ik(x-y)} G(p, k) dp dk \tag{16}$$

where the integrals over p and k_1 are Riemann sums on a $\frac{\pi}{N}$ lattice. The inverse of A_4 is written as

$$-A_4^{-1} = \int_0^\infty e^{tA_4} dt = \int_0^\infty R(t)^{\otimes 4} dt$$

where $R(t) = e^{tA}$. In Fourier space the latter is

$$\widehat{R}(t, q) = \frac{1}{2} \sum_{s=\pm 1} e^{(is\omega(q)-\epsilon)t} \begin{pmatrix} 1 & -is\omega(q)^{-1} \\ is\omega(q) & 1 \end{pmatrix}. \tag{17}$$

Then some algebra yields the following expression for the nonlinear term

$$\begin{aligned} N(p, k) = \sum_{\mathbf{s}} \int dv \Big(\sum_1^4 s_i \omega(p_i + k_i) + i\epsilon \Big)^{-1} \prod_{i=1}^2 W_{s_i}(p_i, k_i) \\ \times \begin{pmatrix} 0 & 0 \\ 1 & is_4\omega(p_4 + k_4) \end{pmatrix} \\ \times s_3 \omega(p_3 + k_3) \big[\omega(p_3 + k_3)^{-2} \delta(2p_3) W_{s_4}(p_4, k_4) \\ - \omega(p_4 + k_4)^{-2} \delta(2p_4) W_{s_3}(p_3, k_3) \big] \end{aligned} \tag{18}$$

where

$$dv = \delta\Big(2p - \sum (p_i + k_i)\Big) \delta\Big(\sum (p_i - k_i)\Big) \delta(p - k - p_4 - k_4) d\mathbf{p} d\mathbf{k}, \tag{19}$$

and $\mathbf{k} = (k_i)_{i=1}^4$ and similarly for $\mathbf{p}$ and $\mathbf{s}$. W is the following combination

$$W_s(p,q) = \widehat{Q}(p,q) + is\omega(p+q)^{-1}\widehat{J}(p,q). \tag{20}$$

4 Kinetic Limit

Equation (14) is a nonlinear set of equations for the pair correlation functions of our model. In [2] we have proven that they have a unique solution which describes a nonlinear temperature profile and leads to Fourier's law in the scaling limit. We will now explain this in a particular scaling limit of our model, the so called kinetic limit where λ is taken to zero with the scaling parameter by writing

$$\lambda^2 = g/N.$$

In this limit (14) simplifies a bit by becoming *local* in the variable $x = x_1 + y_1$. Define the function $V(x,k) = \omega Q(x,k) + iJ(x,k)$, where $x \in [0,1]$ results from a rescaling of the lattice interval $[0,N]$ to the unit interval. Then (14) becomes

$$\nabla\omega(k)\nabla_x V(x,k) = gC(V) \tag{21}$$

with

$$\begin{aligned} C(V) = \frac{9\pi^2}{2}\int dk_1 dk_3 dk_3 (\omega(k)\omega(k_1)\omega(k_2)\omega(k_3))^{-1} \\ \times \delta(\omega(k)+\omega(k_1)-\omega(k_2)-\omega(k_3))\delta(k+k_1-k_2-k_3) \\ \times [V(k_1)V(k_2)V(k_3) - V(k)(V(k_1)V(k_2)+V(k_1)V(k_3) \\ - V(k_3)V(k_3))] \end{aligned} \tag{22}$$

where the integration is over $k_i \in [0,2\pi]^d$. Equation (21) is called the *phonon Boltzmann equation* and is expected to be exact in the kinetic limit of the full Markov process (see [10] for a discussion of the kinetic theory of phonon systems). The nonlinear term $C(V)$ can be interpreted as a collision operator for a gas of phonons i.e. Fourier modes of lattice vibrations. The phonons carry a momentum k and "energy" $\omega(k)$ both of which are conserved in the two body collisions as indicated by the delta functions in (22). The role of the one particle density in the standard Boltzmann equation for gases is here played by V which is related to the covariance of the Gaussian measure describing the stationary state.

Equation (21) has to be equipped with boundary conditions that follow by taking limits of (14) (the friction and source terms produce the boundary conditions). Instead of explaining them (see [7]) here let us rather consider the time dependent problem of approach to equilibrium discussed in Sect. 2 in the kinetic limit with $x \in \mathbb{R}$ i.e. the equation

$$\dot{V} + \nabla\omega(k)\nabla_x V = gC(V). \tag{23}$$

The equilibrium states are solutions to the equation $C(V) = 0$ and come as a two-parameter family:

$$V_{T,A}(x,k) = \frac{T}{\omega(k) + A}. \tag{24}$$

The usual Gaussian Gibbs state corresponds to $A = 0$ and T is the temperature. The parameter A can be interpreted as the phonon chemical potential.

Corresponding to this two parameter family there are two conservation laws in our equation. Indeed, for all V,

$$\int dk C(V)(k) = \int dk \omega(k) C(V)(k) = 0. \tag{25}$$

Let us define, for $\alpha = 0, 1$,

$$j_\alpha(t,x) = -\int dk \omega(k)^\alpha \nabla \omega(k) V(t,x,k). \tag{26}$$

j_1 is the thermal current and j_0 can be called the phonon number current. Similarly, set

$$T_\alpha(t,x) = \int dk \omega(k)^\alpha V(t,x,k). \tag{27}$$

T_1 is the temperature and T_0 is related to the phonon chemical potential. Equations (21) and (25) give then the conservation laws

$$\dot{T}_\alpha = \nabla \cdot j_\alpha. \tag{28}$$

The existence of two conservation laws is an artifact of the kinetic limit (and the closure too) coming from the absence of the connected six point function in our closure equation. Inclusion of that term will remove the phonon number conservation.

T_α are the slow modes that will diffuse and the currents j_α will be fast modes that will be slaved to the gradients of T_α via the Fourier law. Let us see how this comes about by linearizing (23) around an equilibrium solution.

Let $\hat{V}(t, p, k)$ denote the Fourier transform of W in the x variable. We shall look for solutions of (23) of the form:

$$\hat{V}(t, p, k) = V_0(k)\delta(p) + w(t, p, k), \tag{29}$$

where $V_0 = \omega^{-1}$ (we set the equilibrium temperature to one for convenience). Equation (23) becomes then,

$$\dot{w} = -Lw + ip \cdot \nabla \omega(k) w + n(w), \tag{30}$$

where the linear operator is given by

$$L = -DC(V_0) \tag{31}$$

and the nonlinear term is $n(w) = C(V_0 + w) + Lw = C(V_0 + w) - DC(V_0)w$.

Differentiating $0 = C(V_{T,A})$ at $T = A = 0$ we find two zero modes for L:

$$L\omega^{\alpha} = 0$$

for $\alpha = -1, -2$. Define the Hilbert space

$$\mathscr{H} = L^2(\mathbb{T}^d, \omega(k)^2 dk) \tag{32}$$

and let P be the orthogonal projection in $\mathscr{H}$ on $E = \text{span}\{\omega^{-1}, \omega^{-2}\}$ and let Q be the one on the orthogonal complement of E. Then one can show L is strictly positive in E. Thus we should decompose w as $w(t) = T(t) + v(t)$ with

$$Pw = T, \quad Qw = v.$$

The identities (25) can be written as:

$$Pn = 0, \tag{33}$$

or $n = Qn$, since, by differentiation, (25) implies the same identities with $C(V)$ replaced by $DC(V_0)w$. Equation (30) thus becomes

$$\dot{T} = iPp \cdot \nabla\omega(k)v \tag{34}$$

$$\dot{v} = -Lv + ipQ \cdot \nabla\omega(k)T + n(w). \tag{35}$$

We see that v has fast dynamics due to the positivity of L. Hence v is slaved to

$$v_0(t) = iL^{-1}p \cdot \nabla\omega T(t), \tag{36}$$

up to nonlinear corrections and then up to such terms

$$\dot{T} = -p^2\kappa T, \tag{37}$$

where $\kappa : E \to E$ is the linear operator

$$\kappa = P\omega' L^{-1}\omega' P, \tag{38}$$

where $\omega' = \frac{\partial\omega}{\partial k^1}$. κ is strictly positive. The linearization hence leads to a linear diffusion equation for the slow variables T.

Equation (36) in turn implies the Fourier law for the leading terms of the solution. Write T in the basis

$$T(t, p, k) = \sum_{\beta=1,2} \omega^{-\beta}(k)\tilde{T}_{\beta}(t, p), \tag{39}$$

(since the basis is not orthogonal, $\tilde{T}_{\beta}$ does not coincide with the Fourier transform of T_{β} in (27)). Then, in x-space, the currents (26) (where, by symmetry, only the v part of W contributes) become

$$j_\alpha = \sum_\beta \kappa_{\alpha\beta} \nabla \tilde{T}_\beta, \tag{40}$$

with the positive conductivity matrix

$$\kappa_{\alpha\beta} = (\omega^{-\alpha}, \kappa \omega^{-\beta}), \tag{41}$$

with κ given by (38).

This linear analysis captures the leading large time asymptotics of the Boltzmann equation (for proof see [3]), corrections from nonlinear terms are down by $\mathcal{O}(t^{-\frac{1}{2}})$. One can also derive a nonlinear heat equation as the hydrodynamic scaling limit of the Boltzmann equation (23). We scale

$$V(t, x, k) = W(\epsilon^2 t, \epsilon x, k),$$

Then we obtain, for W, the equation:

$$\dot{W}(x, k, t) + \epsilon^{-1} \nabla \omega(k) \cdot \nabla W(x, k, t) = \epsilon^{-2} g C(W)(x, k, t). \tag{42}$$

We shall solve it with initial data $W|_{t=0} = \omega(k)^{-1} + w(x, k, 0)$ and

$$w(x, k, 0) = T(x, k, 0) + \epsilon v(x, k, 0), \tag{43}$$

with $T(x, \cdot, 0) \in E$, $v_0(x, \cdot, 0) \in E^\perp$. $V(x, k, 0) = W(0, \epsilon x, k)$ has spatial variations at scale ϵ^{-1}. One can then show that as $\epsilon \to 0$ the solution to (42) converges in a suitable space to solution of the pair

$$DC(\omega^{-1} + T)v = (2\pi)^{-1} \nabla \omega \cdot \nabla T \tag{44}$$

$$\dot{T} = -(2\pi)^{-1} P \nabla \omega \cdot \nabla v \tag{45}$$

which leads to the nonlinear heat equation

$$\dot{T} = \nabla \cdot (\mathcal{K}(T) \nabla T) \tag{46}$$

with

$$\mathcal{K}(T) = -P\omega' DC(\omega^{-1} + T)^{-1} \omega' P -. \tag{47}$$

The nonlinear conductivity matrix $\mathcal{K}(T)$ is again positive.

The analysis of the stationary state of our closure equation proceeds along similar lines, but this time a stationary x dependent solution emerges. In the scaling limit (44) leads to Fourier's law whereas (46) with appropriate boundary conditions implies a nonlinear temperature (and phonon chemical potential) profile.

In conclusion, the closure equations provide an approximation to the full Hopf equations of the nonequilibrium state that allow us to rigorously show how the Fourier law emerges as the system size gets large. Moreover, this approximation should become exact in the kinetic scaling limit. It is a mathematical challenge to

prove that in the kinetic limit the full system reduces to the Boltzman equation (21). Such results have been previously proven for the harmonic model with random masses for the particles [9], based on earlier work on Schroedinger equation in a random potential [6]. The nonlinear Hamiltonian problem has similar features but is considerably more complex.

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Noncommutative Manifolds and Quantum Groups

Giovanni Landi

Abstract For quite sometime, it has been problematic to endow spaces coming from quantum groups with a noncommutative spin structure and such a possibility has eluded several approaches. We review the constructions of the isospectral equivariant spectral triple on the manifold of quantum $SU(2)$, a paradigm for recent constructions of equivariant spectral triples on a variety of examples that include families of quantum two spheres, as well as higher dimensional quantum spheres.

1 Introduction

The recent constructions of equivariant spectral triples—with the consequent analysis of the corresponding noncommutative spectral geometries—have provided a number of examples showing that a marriage between noncommutative geometry and quantum groups theory is indeed possible. Examples includes the manifold of the quantum $SU(2)$ group in [5, 9] (with "singular" spectral triples) and in [15, 16] (with "isospectral" spectral triples), for its quantum homogeneous spaces, the Podleś spheres, in [13, 27, 30] ("exponential" spectral triples), and in [14, 17, 18] ("isospectral" spectral triples). There are also spectral triples on irreducible quantum flag manifolds [24] as well as for the 4-dimensional quantum orthogonal sphere [19] (an "isospectral" one).

A common feature of the isospectral examples is that while they have all spectral properties as in their commutative limit and are regular, in order to have a real structure one is forced to weaken the usual requirements that such structure should satisfy. The exponential spectral triple proposed in [13] maintains the original requirements for a real spectral triples but sacrifices regularity, as was pointed out in [27]. A general strategy for the construction of isospectral noncommutative geometries

Giovanni Landi
Dipartimento di Matematica e Informatica, Università di Trieste, Via A. Valerio 12/1, 34127 Trieste, Italy and INFN, Sezione di Trieste, Trieste, Italy, e-mail: landi@units.it

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on any quantum group has been very recently given in [28], an outline of the construction being already present in [1]. These constructions do not include yet an analysis of real structures.

In the present report, as an example of the general construction, we review in detail the construction in [15] of the isospectral spectral triple for the quantum group $SU_q(2)$. The possibility of such a triple $(\mathscr{A}(SU_q(2)), \mathscr{H}, D)$ was suggested in [11]. A crucial requirement is that all commutators $[D, x]$, with $x \in \mathscr{A}(SU_q(2))$, must extend to bounded operators on $\mathscr{H}$ as required by the general theory [7]. Counterexamples to boundedness were soon found [20]. This obstacle was later surmounted [15] by the construction of a 3-dimensional noncommutative geometry on the manifold of $SU_q(2)$. For that geometry, the spectrum of the operator D is the same as that of the usual Dirac operator on the 3-sphere $\mathbb{S}^3 \simeq SU(2)$, with it rotation-invariant metric. In this sense the deformation, from $SU(2)$ to $SU_q(2)$, is isospectral, and in particular the metric dimension of the spectral geometry is 3.

The spectral triple of [15] is equivariant with respect to the full symmetry algebra $\mathscr{U}_q(su(2)) \otimes \mathscr{U}_q(su(2))$ of the quantum group manifold $SU_q(2)$: this is implemented as a pair of commuting left and right actions of $\mathscr{U}_q(su(2))$ on the algebra $\mathscr{A} = \mathscr{A}(SU_q(2))$. The equivariance is the crucial requirement for the construction. It allows one to compute from scratch the spin representation of the algebra $\mathscr{A}$, in a form that differs slightly from that of [20]; and it then selects a class of possible "Dirac" operators D. For such an operator D having a classical spectrum, that is, whose eigenvalues depend linearly on the "total angular momentum" and have the correct multiplicities, one prove boundedness of the commutators $[D, x]$, for all $x \in \mathscr{A}$.

An equivariant real structure J is constructed by suitably lifting to the Hilbert space of spinors $\mathscr{H}$ the Tomita conjugation operator for the left regular representation of $\mathscr{A}$. Unlike the Tomita operator for the spin representation, however, this J does not intertwine the spin representation of $\mathscr{A}$ with its commutant. It is thus incompatible with the full set of requirements for a real spectral triple that was proposed in [8] (see also [21]) to define a "noncommutative spin geometry". It turns out that this commutant property, and the companion "first-order" property of D, hold up to infinitesimals of arbitrarily high order.

A different spectral triple for $SU_q(2)$ had already been constructed in [5]; it is however "singular", insofar as it does not admit a commutative limit when $q \to 1$. That geometry was incorporated into the general framework of Connes and Moscovici [12] by a full computation of its local index formula [9]. We review herein a parallel analysis, already achieved in [16], for our isospectral noncommutative geometry on $SU_q(2)$.

In the paper [16], just as in [9], one constructs a "cosphere bundle" $\mathbb{S}^*_q \to SU_q(2)$. In the algebra $\mathscr{B} = \bigcup_{n=0}^{\infty} \delta^n(\mathscr{A})$, where $\delta(T) := [|D|, T]$, an element x is determined, up to smoothing operators—that do not contribute to the residues appearing in the terms of the local index formula—by its "symbol" $\rho(x)$ in the algebra $C^\infty(D^2_{q+} \times D^2_{q-} \times \mathbb{S}^1)$, where $D^2_{q\pm}$ are two quantum disks. The cosphere algebra $C^\infty(\mathbb{S}^*_q)$ is the image under the symbol map ρ of $\mathscr{B}$. By discarding smoothing operators, one computes the dimension spectrum and obtains simple expressions for the residues in the local index formula.

It turns out that for our isospectral geometry the cosphere bundle coincides with the one constructed in [9] to analyse the singular spectral triple of [5]. The dimension spectra of both spectral triples is also the same: it is simple and consists of the set $\{1, 2, 3\}$.

It is known [25] that the cyclic cohomology of $\mathscr{A}(SU_q(2)$ has a single generator; our local index computation allows us to exhibit a representing cocycle in Connes' (b, B)-bicomplex [12]. When compared to that of [9], the cocycle of [16] contains an extra term proportional to $\frac{1}{2}(1 + \mathrm{Sign}\, D)\,|D|^{-3}$. We also show how to compute the Fredholm index pairing of the K-homology class of our $(\mathscr{A}, \mathscr{H}, D)$ with the generator of $K_1(\mathscr{A})$.

In the present report all statements are given without proofs; for these and for additional details we refer to the papers [15] and [16].

2 The Algebras and the Representations

We start with some algebraic preliminaries on the algebras of functions $\mathscr{A} = \mathscr{A}(SU_q(2))$ and of infinitesimal symmetries $\mathscr{U}_q(su(2))$.

2.1 The Algebras of Functions and of Symmetries

Definition 1. For q real, $0 < q < 1$, we denote by $\mathscr{A} = \mathscr{A}(SU_q(2))$ the $*$-algebra generated by elements a and b, subject to the commutation rules

$$\begin{aligned} &ba = qab, \qquad b^*a = qab^*, \qquad bb^* = b^*b, \\ &a^*a + q^2b^*b = 1, \qquad aa^* + bb^* = 1. \end{aligned} \tag{1}$$

The algebra $\mathscr{A}$ comes with a Hopf $*$-algebra structure, with coproduct

$$\Delta a := a \otimes a - q\, b \otimes b^*, \qquad \Delta b := b \otimes a^* + a \otimes b, \tag{2}$$

counit $\varepsilon(a) = 1$, $\varepsilon(b) = 0$, and antipode $Sa = a^*$, $Sb = -qb$, $Sb^* = -q^{-1}b^*$, $Sa^* = a$.

Definition 2. The Hopf $*$-algebra $\mathscr{U} = \mathscr{U}_q(su(2))$ is generated as an algebra by elements e, f, k, with k invertible, satisfying the relations

$$ek = qke, \qquad kf = qfk, \qquad k^2 - k^{-2} = (q - q^{-1})(fe - ef)$$

and involution * given on elements by:

$$k^* = k, \qquad f^* = e, \qquad e^* = f.$$

The coproduct Δ is given by

$$\Delta k = k \otimes k, \qquad \Delta e = e \otimes k + k^{-1} \otimes e, \qquad \Delta f = f \otimes k + k^{-1} \otimes f,$$

while its counit ϵ and antipode S are given respectively by

$$\epsilon(k) = 1, \qquad \epsilon(f) = 0, \qquad \epsilon(e) = 0,$$
$$Sk = k^{-1}, \qquad Sf = -qf, \qquad Se = -q^{-1}e.$$

Definition 3. The canonical duality pairing between $\mathscr{U}$ and $\mathscr{A}$ is defined on generators by

$$\langle k, a \rangle = q^{\frac{1}{2}}, \qquad \langle k, a^* \rangle = q^{-\frac{1}{2}}, \qquad \langle e, -qb^* \rangle = \langle f, b \rangle = 1,$$

with all other couples of generators pairing to 0. It satisfies

$$\langle (Sh)^*, x \rangle = \overline{\langle h, x^* \rangle}, \quad \text{for all } h \in \mathscr{U},\ x \in \mathscr{A}. \tag{3}$$

With this pairing there come [32] canonical left and right $\mathscr{U}$-module algebra structures on $\mathscr{A}$ such that

$$\langle g, h \triangleright x \rangle := \langle gh, x \rangle, \qquad \langle g, x \triangleleft h \rangle := \langle hg, x \rangle, \quad \text{for all } g, h \in \mathscr{U},\ x \in \mathscr{A}.$$

These mutually commuting actions of $\mathscr{U}$ on $\mathscr{A}$ are given by

$$h \triangleright x := (\mathrm{id} \otimes h)\Delta x = x_{(1)} \langle h, x_{(2)} \rangle, \qquad x \triangleleft h := (h \otimes \mathrm{id})\, \Delta x = \langle h, x_{(1)} \rangle x_{(2)},$$

using the Sweedler notation $\Delta x =: x_{(1)} \otimes x_{(2)}$ with implicit summation.

The actions are linked through the antipodes:

$$S(Sh \triangleright x) = Sx \triangleleft h.$$

Also, it follows from (3) that the star structure is compatible with both,

$$h \triangleright x^* = ((Sh)^* \triangleright x)^*, \qquad x^* \triangleleft h = (x \triangleleft (Sh)^*)^*, \quad \text{for all } h \in \mathscr{U},\ x \in \mathscr{A}.$$

It is convenient to convert the right action into a second left action commuting with the first:

$$h \cdot x := x \triangleleft S^{-1}(\vartheta(h)),$$

where the automorphism ϑ of $\mathscr{U}$ is defined on generators by

$$\vartheta(k) := k^{-1}, \qquad \vartheta(f) := -e, \qquad \vartheta(e) := -f; \tag{4}$$

it is an antiautomorphism for the coalgebra structure of $\mathscr{U}$. Since $S^{-1} \circ \vartheta$ is an algebra antiautomorphism of $\mathscr{U}$, it converts a right action into a left action; and

because both S^{-1} and ϑ are coalgebra antiautomorphisms, $S^{-1} \circ \vartheta$ preserves the coalgebra structure of $\mathscr{U}$. Explicitly, both left actions on all generators are:

$$\begin{aligned} &k \triangleright a = q^{\frac{1}{2}} a, && k \triangleright a^* = q^{-\frac{1}{2}} a^*, && k \triangleright b = q^{-\frac{1}{2}} b, && k \triangleright b^* = q^{\frac{1}{2}} b^*, \\ &f \triangleright a = 0, && f \triangleright a^* = -q b^*, && f \triangleright b = a, && f \triangleright b^* = 0, \\ &e \triangleright a = b, && e \triangleright a^* = 0, && e \triangleright b = 0, && e \triangleright b^* = -q^{-1} a^*, \end{aligned}$$

and

$$\begin{aligned} &k \cdot a = q^{\frac{1}{2}} a, && k \cdot a^* = q^{-\frac{1}{2}} a^*, && k \cdot b = q^{\frac{1}{2}} b, && k \cdot b^* = q^{-\frac{1}{2}} b^*, \\ &f \cdot a = 0, && f \cdot a^* = q b, && f \cdot b = 0, && f \cdot b^* = -a, \\ &e \cdot a = -b^*, && e \cdot a^* = 0, && e \cdot b = q^{-1} a^*, && e \cdot b^* = 0. \end{aligned}$$

Together, these give a left action of $\mathscr{U}_q(su(2)) \otimes \mathscr{U}_q(su(2))$ on $\mathscr{A}(SU_q(2))$, that extends to the case $q \neq 1$ the (infinitesimal) classical action of $\mathrm{Spin}(4) = SU(2) \times SU(2)$ on $SU(2) \approx \mathbb{S}^3$, realized as two commuting left actions of $SU(2)$.

Next, we recall [23] that $\mathscr{A} = \mathscr{A}(SU_q(2))$ has a vector-space basis consisting of matrix elements of its irreducible corepresentations, $\{t^l_{mn} : 2l \in \mathbb{N},\ m, n = -l, \ldots, l-1, l\}$, with

$$t^0_{00} = 1, \qquad t^{\frac{1}{2}}_{\frac{1}{2},\frac{1}{2}} = a, \qquad t^{\frac{1}{2}}_{\frac{1}{2},-\frac{1}{2}} = b.$$

The coproduct has the matricial form $\Delta t^l_{mn} = \sum_k t^l_{mk} \otimes t^l_{kn}$, while the product is

$$t^j_{rs} t^l_{mn} = \sum_{k=|j-l|}^{j+l} C_q \begin{pmatrix} j & l & k \\ r & m & r+m \end{pmatrix} C_q \begin{pmatrix} j & l & k \\ s & n & s+n \end{pmatrix} t^k_{r+m,s+n},$$

where the $C_q(-)$ factors are q-Clebsch–Gordan coefficients [3, 22].

The Haar state ψ on the C^*-completion $C(SU_q(2))$ is determined by setting $\psi(1) := 1$ and $\psi(t^l_{mn}) := 0$ if $l > 0$. Let $\mathscr{H}_\psi = L^2(SU_q(2), \psi)$ be the Hilbert space of its GNS representation. The GNS map $\eta\colon C(SU_q(2)) \to \mathscr{H}_\psi$ is injective and satisfies

$$\|\eta(t^l_{mn})\|^2 = \psi((t^l_{mn})^* t^l_{mn}) = \frac{q^{-2m}}{[2l+1]},$$

and the vectors $\eta(t^l_{mn})$ are mutually orthogonal. From the formula

$$C_q \begin{pmatrix} l & l & 0 \\ -m & m & 0 \end{pmatrix} = (-1)^{l+m} \frac{q^{-m}}{[2l+1]^{\frac{1}{2}}},$$

we see that the involution in $C(SU_q(2))$ is given by

$$(t^l_{mn})^* = (-1)^{2l+m+n} q^{n-m}\, t^l_{-m,-n}, \tag{5}$$

and in particular, $t^{\frac{1}{2}}_{-\frac{1}{2},\frac{1}{2}} = -qb^*$ and $t^{\frac{1}{2}}_{-\frac{1}{2},-\frac{1}{2}} = a^*$. An orthonormal basis of $\mathscr{H}_\psi$ is given by

$$|lmn\rangle := q^m[2l+1]^{\frac{1}{2}}\eta(t^l_{mn}). \tag{6}$$

We denote by π_ψ the corresponding GNS representation of $C(SU_q(2))$ on $\mathscr{H}_\psi$,

$$\pi_\psi(x)|lmn\rangle := q^m[2l+1]^{\frac{1}{2}}\,\eta(x\,t^l_{mn}). \tag{7}$$

2.2 The Equivariant Representation of $\mathscr{A}(SU_q(2))$

We shall first outline one way to construct the regular representation of the algebra $\mathscr{A}(SU_q(2))$ on its GNS space $\mathscr{H}_\psi$, showing how it is determined by its equivariance properties with respect to the left Hopf action of $\mathscr{U}\otimes\mathscr{U}$ (for details see [15]).

Definition 4. Let λ and ρ be mutually commuting representations of the Hopf algebra $\mathscr{U}$ on a vector space V. A representation π of the $*$-algebra $\mathscr{A}$ on V is (λ,ρ)-*equivariant* if the following compatibility relations hold:

$$\lambda(h)\,\pi(x)\xi = \pi(h_{(1)}\cdot x)\lambda(h_{(2)})\xi, \qquad \rho(h)\,\pi(x)\xi = \pi(h_{(1)}\triangleright x)\rho(h_{(2)})\xi,$$

for all $h\in\mathscr{U}$, $x\in\mathscr{A}$ and $\xi\in V$.

For the case of $\mathscr{A} = \mathscr{A}(SU_q(2))$, the two $\mathscr{U} = \mathscr{U}_q(su(2))$ symmetries λ and ρ are build from the irreducible (involutive) representations of $\mathscr{U}_q(su(2))$; these are well known [23] and we now recall them. The irreducible $*$-representations σ_l of $\mathscr{U}_q(su(2))$ are labelled by a nonnegative half-integer (the spin) $l = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$, acting on a $\mathscr{U}$-module V_l with $\dim V_l = 2l+1$, and having orthonormal bases $\{|lm\rangle : m = -l, -l+1, \ldots, l-1, l\}$. They are given by

$$\begin{aligned}
\sigma_l(k)\,|lm\rangle &= q^m\,|lm\rangle,\\
\sigma_l(f)\,|lm\rangle &= \sqrt{[l-m][l+m+1]}\,|l,m+1\rangle,\\
\sigma_l(e)\,|lm\rangle &= \sqrt{[l-m+1][l+m]}\,|l,m-1\rangle.
\end{aligned} \tag{8}$$

Here, for each $n\in\mathbb{Z}$, let $[n] =:= (q^n - q^{-n})/(q-q^{-1})$ be the corresponding "q-integer".

The equivariant representation of $\mathscr{A}(SU_q(2))$ we seek acts on the preHilbert space which is the (algebraic) direct sum

$$V := \bigoplus_{2l=0}^{\infty} V_l\otimes V_l,$$

while the symmetries λ and ρ act on the first and the second leg of the tensor product respectively, via the irreps (8):

$$\lambda(h) = \sigma_l(h) \otimes \mathrm{id}, \qquad \rho(h) = \mathrm{id} \otimes \sigma_l(h) \quad \text{on } V_l \otimes V_l. \tag{9}$$

We abbreviate $|lmn\rangle := |lm\rangle \otimes |ln\rangle$, for $m, n = -l, \ldots, l-1, l$. These form an orthonormal basis for $V_l \otimes V_l$, for each fixed l. Also, we adopt a shorthand notation,

$$l^{\pm} := l \pm \frac{1}{2}, \qquad m^{\pm} := m \pm \frac{1}{2}, \qquad n^{\pm} := n \pm \frac{1}{2}.$$

Proposition 5. *A (λ, ρ)-equivariant $*$-representation π of $\mathscr{A}(SU_q(2))$ on V must have the form,*

$$\begin{aligned} \pi(a)|lmn\rangle &= A^{+}_{lmn}|l^{+}m^{+}n^{+}\rangle + A^{-}_{lmn}|l^{-}m^{+}n^{+}\rangle, \\ \pi(b)\,|lmn\rangle &= B^{+}_{lmn}|l^{+}m^{+}n^{-}\rangle + B^{-}_{lmn}|l^{-}m^{+}n^{-}\rangle, \end{aligned} \tag{10}$$

where, up to phase factors depending only on l, the constants $A^{\pm}_{lmn}$ and $B^{\pm}_{lmn}$ are,

$$\begin{aligned} A^{+}_{lmn} &= q^{(-2l+m+n-1)/2}\left(\frac{[l+m+1][l+n+1]}{[2l+1][2l+2]}\right)^{\frac{1}{2}}, \\ A^{-}_{lmn} &= q^{(2l+m+n+1)/2}\left(\frac{[l-m][l-n]}{[2l][2l+1]}\right)^{\frac{1}{2}}, \\ B^{+}_{lmn} &= q^{(m+n-1)/2}\left(\frac{[l+m+1][l-n+1]}{[2l+1][2l+2]}\right)^{\frac{1}{2}}, \\ B^{-}_{lmn} &= -q^{(m+n-1)/2}\left(\frac{[l-m][l+n]}{[2l][2l+1]}\right)^{\frac{1}{2}}. \end{aligned} \tag{11}$$

As shown in [15] (and as already noted in [5]), the formulae (10) and (11) give precisely the left regular representation π_ψ of $\mathscr{A}(SU_q(2))$ in (7). The identification (6) embeds the preHilbert space V densely in the Hilbert space $\mathscr{H}_\psi$, and the representation π_ψ extends to the GNS representation of $C(SU_q(2))$ on $\mathscr{H}_\psi$, as described by the Peter–Weyl theorem [23, 32]. In a similar manner, all other representations of $\mathscr{A}$ given in this paper extend to C^*-algebra representations of $C(SU_q(2))$ on the appropriate Hilbert spaces.

2.3 The Spin Representation

Definition 6. The left regular representation π of $\mathscr{A}$ on V is amplified to $\pi' = \pi \otimes \mathrm{id}$ on $W := V \otimes \mathbb{C}^2 = V \otimes V_{\frac{1}{2}}$.

In the commutative case when $q = 1$, this yields the spinor representation of $SU(2)$, because the spinor bundle is parallelizable: $S \simeq SU(2) \times \mathbb{C}^2$, although one needs to specify the trivialization. The representation theory of $\mathscr{U}$ (and the corepresentation theory of $\mathscr{A}$) follows the same pattern; when $q \neq 1$ only the Clebsch–

Gordan coefficients need to be modified [22]. The Clebsch–Gordan decomposition of W is the (algebraic) direct sum

$$W = \left(\bigoplus_{2l=0}^{\infty} V_l \otimes V_l\right) \otimes V_{\frac{1}{2}} \simeq V_{\frac{1}{2}} \oplus \bigoplus_{2j=1}^{\infty} (V_{j+\frac{1}{2}} \otimes V_j) \oplus (V_{j-\frac{1}{2}} \otimes V_j)$$
$$= W_0^{\uparrow} \oplus \bigoplus_{2j\geq 1} W_j^{\uparrow} \oplus W_j^{\downarrow}, \tag{12}$$

with

$$W_j^{\uparrow} \simeq V_{j+\frac{1}{2}} \otimes V_j, \qquad \dim W_j^{\uparrow} = (2j+1)(2j+2), \quad \text{for } j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots,$$
$$W_j^{\downarrow} \simeq V_{j-\frac{1}{2}} \otimes V_j, \qquad \dim W_j^{\downarrow} = 2j(2j+1), \quad \text{for } j = \frac{1}{2}, 1, \frac{3}{2}, \ldots.$$

Definition 7. We amplify the representation ρ of $\mathscr{U}$ on V to $\rho' = \rho \otimes \mathrm{id}$ on $W = V \otimes \mathbb{C}^2$. However, we replace λ on V by its tensor product with $\sigma_{\frac{1}{2}}$ on $\mathbb{C}^2$,

$$\lambda'(h) := (\lambda \otimes \sigma_{\frac{1}{2}})(\Delta h) = \lambda(h_{(1)}) \otimes \sigma_{\frac{1}{2}}(h_{(2)}).$$

It is straightforward to check that the representations λ' and ρ' on W commute, and that the representation π' of $\mathscr{A}$ on W is (λ', ρ')-equivariant:

$$\lambda'(h)\,\pi'(x)\psi = \pi'(h_{(1)} \cdot x)\,\lambda'(h_{(2)})\psi, \qquad \rho'(h)\,\pi'(x)\psi = \pi'(h_{(1)} \triangleright x)\,\rho'(h_{(2)})\psi,$$

for all $h \in \mathscr{U}$, $x \in \mathscr{A}$ and $\psi \in W$.

The spinor Hilbert space $\mathscr{H} := \mathscr{H}_\psi \otimes \mathbb{C}^2$ is just the completion of W. It can be decomposed as $\mathscr{H} = \mathscr{H}^{\uparrow} \oplus \mathscr{H}^{\downarrow}$, where $\mathscr{H}^{\uparrow}$ and $\mathscr{H}^{\downarrow}$ are the respective completions of $\bigoplus_{2j\geq 0} W_j^{\uparrow}$ and $\bigoplus_{2j\geq 1} W_j^{\downarrow}$. An explicit basis, well-adapted to (λ', ρ')-equivariance, is given as follows.

For $j = l + \frac{1}{2}$, $\mu = m - \frac{1}{2}$, with $\mu = -j, \ldots, j$ and $n = -j^-, \ldots, j^-$, let

$$|j\mu n\downarrow\rangle := C_{j\mu}|j^-\mu^+ n\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle + S_{j\mu}|j^-\mu^- n\rangle \otimes \left|\frac{1}{2}, +\frac{1}{2}\right\rangle; \tag{13a}$$

and for $j = l - \frac{1}{2}$, $\mu = m - \frac{1}{2}$, with $\mu = -j, \ldots, j$ and $n = -j^+, \ldots, j^+$, let

$$|j\mu n\uparrow\rangle := -S_{j+1,\mu}\,|j^+\mu^+ n\rangle \otimes \left|\frac{1}{2}, -\frac{1}{2}\right\rangle + C_{j+1,\mu}|j^+\mu^- n\rangle \otimes \left|\frac{1}{2}, +\frac{1}{2}\right\rangle, \tag{13b}$$

where the coefficients are

$$C_{j\mu} := q^{-(j+\mu)/2}\,\frac{[j-\mu]^{\frac{1}{2}}}{[2j]^{\frac{1}{2}}}, \qquad S_{j\mu} := q^{(j-\mu)/2}\,\frac{[j+\mu]^{\frac{1}{2}}}{[2j]^{\frac{1}{2}}}. \tag{13c}$$

Notice that there are no $\downarrow$ vectors for $j = 0$. It is straightforward to verify that these vectors make up orthonormal bases for $W_j^{\downarrow}$ and $W_j^{\uparrow}$, respectively.

The vectors $|j\mu n\uparrow\rangle$ and $|j\mu n\downarrow\rangle$ are joint eigenvectors for $\lambda'(k)$ and $\rho'(k)$, and e, f are represented on them as ladder operators which can be obtained explicitly from Definition 7 and (9) and (8) with the use of the basis transformation (13).

The representation π' can be computed in the new spinor basis by conjugating the form of $\pi \otimes \mathrm{id}$ found in Proposition 5 by the basis transformation (13). It can also be derived directly from the (λ', ρ')-equivariance.

Definition 8. For $j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$, with $\mu = -j, \ldots, j$ and $n = -j - \frac{1}{2}, \ldots, j + \frac{1}{2}$, we juxtapose the pair of spinors

$$|j\mu n\rangle\!\rangle := \begin{pmatrix} |j\mu n\uparrow\rangle \\ |j\mu n\downarrow\rangle \end{pmatrix},$$

with the convention that the lower component is zero when $n = \pm(j + \frac{1}{2})$ or $j = 0$. Furthermore, a matrix with scalar entries,

$$A = \begin{pmatrix} A_{\uparrow\uparrow} & A_{\uparrow\downarrow} \\ A_{\downarrow\uparrow} & A_{\downarrow\downarrow} \end{pmatrix},$$

is understood to act on $|j\mu n\rangle\!\rangle$ by the rule:

$$A|j\mu n\uparrow\rangle = A_{\uparrow\uparrow}|j\mu n\uparrow\rangle + A_{\downarrow\uparrow}|j\mu n\downarrow\rangle,$$

$$A|j\mu n\downarrow\rangle = A_{\downarrow\downarrow}|j\mu n\downarrow\rangle + A_{\uparrow\downarrow}|j\mu n\uparrow\rangle.$$

Proposition 9. *The spinor representation $\pi' := \pi \otimes \mathrm{id}$ of $\mathscr{A}$ on $\mathscr{H}$ is the $*$-representation written as*

$$\pi(a) := a_+ + a_-, \qquad \pi(b) := b_+ + b_-, \tag{14}$$

where $a_\pm$ and $b_\pm$ are, up to phase factors depending only on j, the triangular operators,

$$a_+|j\mu n\rangle\!\rangle$$
$$:= q^{(\mu+n-\frac{1}{2})/2}[j+\mu+1]^{\frac{1}{2}} \begin{pmatrix} q^{-j-\frac{1}{2}}\frac{[j+n+\frac{3}{2}]^{1/2}}{[2j+2]} & 0 \\ q^{\frac{1}{2}}\frac{[j-n+\frac{1}{2}]^{1/2}}{[2j+1][2j+2]} & q^{-j}\frac{[j+n+\frac{1}{2}]^{1/2}}{[2j+1]} \end{pmatrix} |j^+\mu^+n^+\rangle\!\rangle,$$

$$a_-|j\mu n\rangle\!\rangle$$
$$:= q^{(\mu+n-\frac{1}{2})/2}[j-\mu]^{\frac{1}{2}} \begin{pmatrix} q^{j+1}\frac{[j-n+\frac{1}{2}]^{1/2}}{[2j+1]} & -q^{\frac{1}{2}}\frac{[j+n+\frac{1}{2}]^{1/2}}{[2j][2j+1]} \\ 0 & q^{j+\frac{1}{2}}\frac{[j-n-\frac{1}{2}]^{1/2}}{[2j]} \end{pmatrix} |j^-\mu^+n^+\rangle\!\rangle,$$

$$
\begin{aligned}
&b_+|j\mu n\rangle\!\rangle \\
&\quad := q^{(\mu+n-\frac{1}{2})/2}[j+\mu+1]^{\frac{1}{2}} \begin{pmatrix} \frac{[j-n+\frac{3}{2}]^{1/2}}{[2j+2]} & 0 \\ -q^{-j-1}\frac{[j+n+\frac{1}{2}]^{1/2}}{[2j+1][2j+2]} & q^{-\frac{1}{2}}\frac{[j-n+\frac{1}{2}]^{1/2}}{[2j+1]} \end{pmatrix} \\
&\qquad \times |j^+\mu^+n^-\rangle\!\rangle, \\
&b_-|j\mu n\rangle\!\rangle \\
&\quad := q^{(\mu+n-\frac{1}{2})/2}[j-\mu]^{\frac{1}{2}} \begin{pmatrix} -q^{-\frac{1}{2}}\frac{[j+n+\frac{1}{2}]^{1/2}}{[2j+1]} & -q^{j}\frac{[j-n+\frac{1}{2}]^{1/2}}{[2j][2j+1]} \\ 0 & -\frac{[j+n-\frac{1}{2}]^{1/2}}{[2j]} \end{pmatrix} |j^-\mu^+n^-\rangle\!\rangle.
\end{aligned}
\tag{15}
$$

3 The Equivariant Dirac Operator

The central Casimir element of $\mathscr{U}_q(su(2))$ is $C_q = qk^2 + q^{-1}k^{-2} + (q-q^{-1})^2 ef$. The symmetric operators $\lambda'(C_q)$ and $\rho'(C_q)$ on $\mathscr{H}$, having dense domain W, extend to selfadjoint operators on $\mathscr{H}$ and the finite-dimensional subspaces $W_j^{\uparrow}$, $W_j^{\downarrow}$ are their joint eigenspaces,

$$
\begin{aligned}
\lambda'(C_q)|j\mu n\uparrow\rangle &= (q^{2j+1} + q^{-2j-1})|j\mu n\uparrow\rangle, \\
\rho'(C_q)|j\mu n\uparrow\rangle &= (q^{2j+2} + q^{-2j-2})|j\mu n\uparrow\rangle, \\
\lambda'(C_q)|j\mu n\downarrow\rangle &= (q^{2j+1} + q^{-2j-1})|j\mu n\downarrow\rangle, \\
\rho'(C_q)|j\mu n\downarrow\rangle &= (q^{2j} + q^{-2j})|j\mu n\downarrow\rangle.
\end{aligned}
$$

The finite-dimensional subspaces $W_j^{\uparrow}$ and $W_j^{\downarrow}$ will reduce any selfadjoint operator D on $\mathscr{H}$ which commutes strongly with $\lambda'(C_q)$ and $\rho'(C_q)$. If we require that D be invariant under the actions λ' and ρ' of $\mathscr{U}$, we get the following stronger condition.

Lemma 10. *Let D be a selfadjoint operator that commutes strongly with $\lambda'(h)$ and $\rho'(h)$, for each $h \in \mathscr{U}$. Then the subspaces $W_j^{\uparrow}$ and $W_j^{\downarrow}$ are eigenspaces for D,*

$$
D|j\mu n\uparrow\rangle = d_j^{\uparrow}|j\mu n\uparrow\rangle, \qquad D|j\mu n\downarrow\rangle = d_j^{\downarrow}|j\mu n\downarrow\rangle, \tag{16}
$$

where $d_j^{\uparrow}$ and $d_j^{\downarrow}$ are real eigenvalues of D which depend only on j. Their respective multiplicities are $(2j+1)(2j+2)$ and $2j(2j+1)$.

Additional natural restrictions on the eigenvalues $d_j^{\uparrow}, d_j^{\downarrow}$ of the operator D will come from the crucial requirement of boundedness of the commutators $[D, \pi'(x)]$ for $x \in \mathscr{A}$. For instance, take $x = a$. A straightforward computation shows that

$$
\begin{aligned}
[D,\pi'(a)]|j\mu n\uparrow\rangle &= \sum_{\pm}\alpha^{\pm}_{j\mu n\uparrow\uparrow}(d^{\uparrow}_{j^{\pm}}-d^{\uparrow}_{j})|j^{\pm}\mu^{+}n^{+}\uparrow\rangle \\
&\quad+\alpha^{+}_{j\mu n\downarrow\uparrow}(d^{\downarrow}_{j^{+}}-d^{\uparrow}_{j})|j^{+}\mu^{+}n^{+}\downarrow\rangle, \\
[D,\pi'(a)]|j\mu n\downarrow\rangle &= \sum_{\pm}\alpha^{\pm}_{j\mu n\downarrow\downarrow}(d^{\downarrow}_{j^{\pm}}-d^{\downarrow}_{j})|j^{\pm}\mu^{+}n^{+}\downarrow\rangle \\
&\quad+\alpha^{-}_{j\mu n\uparrow\downarrow}(d^{\uparrow}_{j^{-}}-d^{\downarrow}_{j})|j^{-}\mu^{+}n^{+}\uparrow\rangle. \qquad (17)
\end{aligned}
$$

The "q-Dirac" operator D proposed in [2] corresponds to taking, in our notation,

$$d^{\uparrow}_{j}=\frac{2\,[2j+1]}{q+q^{-1}},\qquad d^{\downarrow}_{j}=-d^{\uparrow}_{j}.$$

These are q-analogues of the classical eigenvalues of $\not{D}-\frac{1}{2}$ where $\not{D}$ is the classical Dirac operator on the sphere $\mathbb{S}^3$ (with the round metric). For this particular choice it follows directly from the explicit form (15) of the matrices $\alpha^{\pm}_{j\mu n}$ that the right hand sides of (17) diverge, and therefore $[D,\pi'(a)]$ is unbounded. This fact was already noted in [11] and it was suggested that one should instead consider an operator D whose spectrum is just that of the classical Dirac operator $\not{D}$.

Proposition 11. *Let D be any selfadjoint operator with eigenspaces $W^{\uparrow}_{j}$ and $W^{\downarrow}_{j}$, and eigenvalues (16). If the eigenvalues $d^{\uparrow}_{j}$ and $d^{\downarrow}_{j}$ are linear in j,*

$$d^{\uparrow}_{j}=c^{\uparrow}_{1}j+c^{\uparrow}_{2},\qquad d^{\downarrow}_{j}=c^{\downarrow}_{1}j+c^{\downarrow}_{2}, \qquad (18)$$

with $c^{\uparrow}_{1}$, $c^{\uparrow}_{2}$, $c^{\downarrow}_{1}$, $c^{\downarrow}_{2}$ not depending on j, then $[D,\pi'(x)]$ is a bounded operator for all $x\in\mathscr{A}$.

A selfadjoint operator D as in Proposition 11 is essentially the only possibility for a Dirac operator satisfying a (modified) first-order condition. It is necessary that we assume $c^{\downarrow}_{1}c^{\uparrow}_{1}<0$ in order that the sign of the operator D be nontrivial; but up to irrelevant scaling factors the choice of $c^{\uparrow}_{j}$ and $c^{\downarrow}_{j}$ is otherwise immaterial. With the particular choice

$$d^{\uparrow}_{j}=2j+\frac{3}{2},\qquad d^{\downarrow}_{j}=-2j-\frac{1}{2}, \qquad (19)$$

the spectrum of D, with multiplicity, coincides with that of the classical Dirac operator $\not{D}$ on the round sphere $\mathbb{S}^3$. Thus, we can regard our spectral triple as an isospectral deformation of $(C^{\infty}(\mathbb{S}^3),\mathscr{H},\not{D})$, and in particular, its spectral dimension is 3.

We let $D=F|D|$ be the polar decomposition of D. Explicitly,

$$F|j\mu n\rangle\!\rangle=\begin{pmatrix}1&0\\0&-1\end{pmatrix}|j\mu n\rangle\!\rangle,\qquad |D|\,|j\mu n\rangle\!\rangle=\begin{pmatrix}2j+\frac{3}{2}&0\\0&2j+\frac{1}{2}\end{pmatrix}|j\mu n\rangle\!\rangle.$$

Then, $P^{\uparrow}:=\frac{1}{2}(1+F)$ and $P^{\downarrow}:=\frac{1}{2}(1-F)=1-P^{\uparrow}$ are the orthogonal projectors whose range spaces are $\mathscr{H}^{\uparrow}$ and $\mathscr{H}^{\downarrow}$, respectively.

With the particular choice of the classical eigenvalues (19) it is also easy to prove regularity. Recall that a spectral triple is called *regular* (see for instance [4, 12, 21]) if the algebra generated by both $\mathscr{A}$ and $[D, \mathscr{A}]$ lie within the smooth domain $\bigcap_{n=0}^{\infty} \mathrm{Dom}\, \delta^n$ of the operator derivation $\delta(T) := |D|T - T|D|$.

The proof of regularity is simplified by observing that the triangular matrix components of the operators $a_\pm$ and $b_\pm$ in (14) give diagonal matrices for $\delta(a_\pm)$ and $\delta(b_\pm)$. Indeed, we get the following operator relations:

$$\begin{aligned} \delta(a_+) &= P^\uparrow a_+ P^\uparrow + P^\downarrow a_+ P^\downarrow, \\ \delta(a_-) &= -P^\uparrow a_- P^\uparrow - P^\downarrow a_- P^\downarrow, \end{aligned} \tag{20a}$$

$$\begin{aligned} \delta([D, a_+]) &= P^\uparrow a_+ P^\uparrow - P^\downarrow a_+ P^\downarrow, \\ \delta([D, a_-]) &= P^\uparrow a_- P^\uparrow - P^\downarrow a_- P^\downarrow, \end{aligned} \tag{20b}$$

together with identical formulae when a is replaced by b.

We summarize our conclusions in the following theorem.

Theorem 12. *The triple $(\mathscr{A}(SU_q(2)), \mathscr{H}, D)$, where the eigenvalues of D are the classical ones given by (19), is a regular 3^+-summable spectral triple.*

4 The Real Structure

For the manifold of $SU_q(2)$, it is shown in [15] that by adding an equivariant real structure J it is not possible to satisfy all usual properties of a real spectral triple like in [8] or [21]. The commutant properties: that J intertwines a left action and a commuting right action of the algebra on the spinor Hilbert space; and the first order condition on D: that the commutators $[D, a]$, for any element a in the algebra, commute with the opposite action by any b, are satisfied only up to a certain ideal of compact operators.

4.1 The Tomita Operator of the Regular Representation

On the GNS representation space $\mathscr{H}_\psi$, the natural involution $T_\psi : \eta(x) \mapsto \eta(x^*)$, is an unbounded (antilinear) operator on $\mathscr{H}_\psi$ with domain $\eta(C(SU_q(2)))$. From the Tomita–Takesaki theory [31], its closure has a polar decomposition $T_\psi =: J_\psi \Delta_\psi^{1/2}$ which defines both the positive "modular operator" Δ_ψ and the antiunitary "modular conjugation" J_ψ. From (5) and (6) it follows that

$$T_\psi \, |lmn\rangle = (-1)^{2l+m+n} q^{m+n} \, |l, -m, -n\rangle,$$

and the adjoint antilinear operator is given by

$$T_\psi^* \,|lmn\rangle = (-1)^{2l+m+n} q^{-m-n} \,|l, -m, -n\rangle.$$

Since $\Delta_\psi = T_\psi^* T_\psi$, it follows that every vector $|lmn\rangle$ lies in the domain Dom Δ_ψ with $\Delta_\psi \,|lmn\rangle = q^{2m+2n} \,|lmn\rangle$. Consequently,

$$J_\psi \,|lmn\rangle = (-1)^{2l+m+n} \,|l, -m, -n\rangle.$$

It is clear that $J_\psi^2 = 1$ on $\mathscr{H}_\psi$. Similar conclusions were already obtained in [6].

Definition 13. Let $\pi^\circ(x) := J_\psi \,\pi(x^*)\, J_\psi^{-1}$, so that π° is a $*$-antirepresentation of $\mathscr{A}$ on $\mathscr{H}_\psi$. Equivalently, π° is a $*$-representation of the opposite algebra $\mathscr{A}(SU_{1/q}(2))$. By Tomita's theorem [31], π and π° are commuting representations.

The (λ, ρ)-equivariance of π is reflected in an analogous equivariance condition for π°.

Lemma 14. *The symmetry of the antirepresentation π° of $\mathscr{A}$ on $\mathscr{H}_\psi$ is given by the equivariance conditions,*

$$\lambda(h)\,\pi^\circ(x)\xi = \pi^\circ(\tilde{h}_{(2)} \cdot x)\,\lambda(h_{(1)})\xi, \qquad \rho(h)\,\pi^\circ(x)\xi = \pi^\circ(\tilde{h}_{(2)} \triangleright x)\,\rho(h_{(1)})\xi,$$

for all $h \in \mathscr{U}$, $x \in \mathscr{A}$ and $\xi \in \mathscr{H}_\psi$. Here $h \mapsto \tilde{h}$ is the automorphism of $\mathscr{U}$ determined on generators by $\tilde{k} := k$, $\tilde{f} := q^{-1} f$, and $\tilde{e} := qe$.

Recall that $T_\psi \eta(x) = \eta(x^*)$ for all $x \in \mathscr{A}$ and that $\eta(x) = \pi(x)\,|000\rangle$. From Definition 4 one finds that for generators h of $\mathscr{U}$,

$$T_\psi \lambda(h)\pi(x)\,|000\rangle = \pi(x^* \triangleleft \vartheta(h)^*)\,|000\rangle = \lambda(S(h)^*) T_\psi \pi(x)\,|000\rangle,$$

where we have used the relation $S(\vartheta(h)^*) = \vartheta(S(h)^*)$. Since the vector $|000\rangle$ is separating for the GNS representation, we conclude that

$$T_\psi \,\lambda(h) T_\psi^{-1} = \lambda((Sh)^*).$$

Similarly, we find that $T_\psi \,\rho(h)\, T_\psi^{-1} = \rho((Sh)^*)$. Thus, the antilinear involutory automorphism $h \mapsto (Sh)^*$ of the Hopf $*$-algebra $\mathscr{U}$ is implemented by the Tomita operator for the Haar state of the dual Hopf $*$-algebra $\mathscr{A}$. This is a known feature of quantum-group duality in the C^*-algebra framework [26].

4.2 The Real Structure on Spinors

The first step in defining an operator J on spinors is to construct the "right multiplication" representation of $\mathscr{A}$ on spinors from its symmetry alone, in close parallel with the equivariance conditions (14) for the right regular representation π° of $\mathscr{A}$ on $\mathscr{H}_\psi$. Then, the conjugation operator J on spinors is constructed as the one that intertwines the left and the right spinor representations.

Proposition 15. *Let π'° be an antirepresentation of $\mathscr{A}$ on $\mathscr{H} = \mathscr{H}_\psi \oplus \mathscr{H}_\psi$ satisfying the following equivariance conditions*:

$$\lambda'(h)\,\pi'^{\circ}(x)\xi = \pi'^{\circ}(\tilde{h}_{(2)}\cdot x)\,\lambda'(h_{(1)})\xi, \qquad \rho'(h)\,\pi'^{\circ}(x)\xi = \pi'^{\circ}(\tilde{h}_{(2)}\triangleright x)\,\rho'(h_{(1)})\xi.$$

Then, up to some phase factors depending only on the index j in the decomposition (12)*, π'° is given on the spinor basis by $\pi'^{\circ}(a) = a^{\circ}_{+} + a^{\circ}_{-}$ and $\pi'^{\circ}(b) = b^{\circ}_{+} + b^{\circ}_{-}$, where in direct analogy with* (14)*, the operators $a^{\circ}_{\pm}$ and $b^{\circ}_{\pm}$ have the triangular-matrix form of* (15)*, acting on the same respective basis vectors: but with the coefficients of $a_{\pm}$ modified by the replacement $q \mapsto q^{-1}$, while the coefficients of $b_{\pm}$ are modified by the replacement $q \mapsto q^{-1}$ and by multiplying the result by an overall factor q^{-1}.*

Definition 16. The conjugation operator J is the antilinear operator on $\mathscr{H}$ defined explicitly on the orthonormal spinor basis by

$$\begin{aligned} J\,|j\mu n\uparrow\rangle &:= i^{2(2j+\mu+n)}\,|j,-\mu,-n,\uparrow\rangle,\\ J\,|j\mu n\downarrow\rangle &:= i^{2(2j-\mu-n)}\,|j,-\mu,-n,\downarrow\rangle. \end{aligned} \tag{21}$$

Such a J is antiunitary and $J^2 = -1$, since each $4j \pm 2(\mu + n)$ is an odd integer.

Proposition 17. *The antiunitary operator J intertwines the left and right spinor representations*:

$$J\,\pi'(x^*)\,J^{-1} = \pi'^{\circ}(x), \quad \text{for all } x \in \mathscr{A}.$$

A minimal requirement for $(\mathscr{A}(SU_q(2)), \mathscr{H}, D, J)$ to constitute a (3^+-summable) real spectral triple is that D and J commute. For the invariant operator D of Sect. 3 this easily follows from the diagonal form of both D and J on their common eigenspaces $W_j^{\uparrow}$ and $W_j^{\downarrow}$, given by the respective equations (16) and (21).

Proposition 18. *The invariant operator D of* (16) *commutes with the conjugation operator J of* (21)*,*

$$J D J^{-1} = D. \tag{22}$$

The conjugation operator J defined by (21) is *not* the Tomita modular conjugation for the spinor representation of $\mathscr{A}$, a fact having consequences on some of the requirements for a real spectral triple, as we shall see presently. The Tomita operator for spinor is $J_\psi \oplus J_\psi$, which does not have a diagonal form in our chosen spinor basis (unless $q = 1$). As mentioned above, conjugation of $\pi'(\mathscr{A}(SU_q(2)))$ by the modular operator would yield a representation of the opposite algebra $\mathscr{A}(SU_{1/q}(2))$, and the commutation relation analogous to (22) would then require D to be equivariant under the corresponding symmetry of $U_{1/q}(su(2))$ say (λ'', ρ''). This extra equivariance condition would force D to be merely a scalar operator, thereby negating the possibility of an equivariant 3^+-summable real spectral triple on $\mathscr{A}(SU_q(2))$ with the modular conjugation operator.

The remedy, in order to get a nontrivial Dirac operator, is to modify J to a non-Tomita conjugation operator. The price to pay for this is that the conditions for a real

spectral triple must be weakened: these are only satisfied up to certain trace-class operators.

Indeed, both the commutant property and the first-order condition of the real spectral triple $(\mathscr{A}(SU_q(2)), \mathscr{H}, D, J)$, are satisfied modulo infinitesimals of arbitrary high order.

For this, it is useful to replace the spinor representation π' of $\mathscr{A}$ of Proposition 9 by a suitable 'approximate representation' $\underline{\pi}'\colon \mathscr{A} \to \mathscr{B}(\mathscr{H})$, such that $\pi'(x) - \underline{\pi}'(x)$ is a compact operator for each $x \in \mathscr{A}$. Although $\underline{\pi}'$ need not preserve the algebra relations of $\mathscr{A}$, the mappings π' and $\underline{\pi}'$ define the same $*$-homomorphism of $\mathscr{A}$ into the Calkin algebra $\mathscr{B}(\mathscr{H})/\mathscr{K}(\mathscr{H})$. We refer to [15] for details, while only mentioning the final results.

Definition 19. We denote by $\mathscr{K}_q$ be the two-sided ideal of $\mathscr{B}(\mathscr{H})$ generated by the positive trace-class operators L_q given by

$$L_q|j\mu n\rangle\!\rangle := q^j\,|j\mu n\rangle\!\rangle \quad \text{for } j \in \frac{1}{2}\mathbb{N}.$$

The ideal $\mathscr{K}_q$ is contained in the ideal of infinitesimals of order α, that is, compact operators whose n-th singular value μ_n satisfies $\mu_n = O(n^{-\alpha})$, for all $\alpha > 0$.

Theorem 20. *The real spectral triple $(\mathscr{A}(SU_q(2)), \mathscr{H}, D, J)$, with $\mathscr{A}(SU_q(2))$ acting on $\mathscr{H}$ via the spinor representation π' of Proposition 9, satisfies both the commutant property and the first order condition up to infinitesimals,*

$$\begin{aligned} [\pi'^{\circ}(x), \pi'(y)] &\in \mathscr{K}_q, \\ [\pi'^{\circ}(x), [D, \pi'(y)]] &\in \mathscr{K}_q, \end{aligned} \quad \textit{for all } x, y \in \mathscr{A}(SU_q(2)).$$

5 The Local Index Formula for $SU_q(2)$

Let $\Psi^0(\mathscr{A})$ be the algebra generated by $\delta^k(\mathscr{A})$ and $\delta^k([D, \mathscr{A}])$ for all $k \geq 0$; it can be thought of as an algebra of pseudodifferential operators of order at most 0. From (20a),

$$\begin{aligned} P^{\uparrow}\pi(a)P^{\uparrow} &= \frac{1}{2}\delta^2(\pi(a)) + \frac{1}{2}\delta([D, \pi(a)]), \\ P^{\uparrow}a_+P^{\uparrow} &= \frac{1}{2}P^{\uparrow}\pi(a)P^{\uparrow} + \frac{1}{2}P^{\uparrow}\delta(\pi(a))P^{\uparrow}, \end{aligned}$$

so the algebra $\Psi^0(\mathscr{A})$ is actually generated by the diagonal operators $P^{\uparrow}a_{\pm}P^{\uparrow}$, $P^{\downarrow}a_{\pm}P^{\downarrow}$, $P^{\uparrow}b_{\pm}P^{\uparrow}$, $P^{\downarrow}b_{\pm}P^{\downarrow}$ together with the off-diagonal operators $P^{\downarrow}a_+P^{\uparrow}$, $P^{\uparrow}a_-P^{\downarrow}$, $P^{\downarrow}b_+P^{\uparrow}$, and $P^{\uparrow}b_-P^{\downarrow}$. Let $\mathscr{B}$ be the subalgebra of $\Psi^0(\mathscr{A})$ generated by all $\delta^k(\mathscr{A})$ for $k \geq 0$. A set of algebra generators are the diagonal operators

$$\tilde{a}_{\pm} := \pm\delta(a_{\pm}) = P^{\uparrow}a_{\pm}P^{\uparrow} + P^{\downarrow}a_{\pm}P^{\downarrow}, \quad \tilde{b}_{\pm} := \pm\delta(b_{\pm}) = P^{\uparrow}b_{\pm}P^{\uparrow} + P^{\downarrow}b_{\pm}P^{\downarrow},$$

together with the off-diagonal operators

$$a_{/} := P^{\downarrow} a_{+} P^{\uparrow} + P^{\uparrow} a_{-} P^{\downarrow}, \qquad b_{/} := P^{\downarrow} b_{+} P^{\uparrow} + P^{\uparrow} b_{-} P^{\downarrow}.$$

5.1 The Cosphere Bundle and the Dimension Spectrum

Much in the same way as done in [9] we now construct Connes' "cosphere bundle" from the spin representation. We first need the two well-known infinite-dimensional representations $\pi_{\pm}$ of $\mathscr{A}(SU_q(2))$ by bounded operators. On the Hilbert space $\ell^2(\mathbb{N})$ with standard orthonormal basis $\{\varepsilon_x : x \in \mathbb{N}\}$, they are given by

$$\pi_{\pm}(a)\,\varepsilon_x := \sqrt{1 - q^{2x+2}}\,\varepsilon_{x+1}, \qquad \pi_{\pm}(b)\,\varepsilon_x := \pm q^x\,\varepsilon_x. \tag{23}$$

They are not faithful on $\mathscr{A}(SU_q(2))$ since $b - b^* \in \ker \pi_{\pm}$. The corresponding quotients,

$$0 \to \ker \pi_{\pm} \to \mathscr{A}(SU_q(2)) \xrightarrow{r_{\pm}} \mathscr{A}(D^2_{q\pm}) \to 0, \tag{24}$$

define two algebras $\mathscr{A}(D^2_{q\pm})$ which may be thought of as quantum disks. Let us omit the quotient maps symbol $r_{\pm}$ for the moment. Then $b = b^*$ in $\mathscr{A}(D^2_{q\pm})$, and the defining relations (1) of $\mathscr{A}(SU_q(2))$ yields

$$ba = q\,ab, \qquad a^*b = q\,ba^*,$$
$$a^*a + q^2b^2 = 1, \qquad aa^* + b^2 = 1.$$

These algebraic relations define two isomorphic quantum 2-spheres $\mathbb{S}^2_{q+} \simeq \mathbb{S}^2_{q-} =: \mathbb{S}^2_q$ which have a classical subspace $\mathbb{S}^1$ given by the characters $b \mapsto 0$, $a \mapsto \lambda$ with $|\lambda| = 1$. A substitution $q \mapsto q^2$, followed by $b \mapsto q^{-2}b$ shows that $\mathbb{S}^2_q$ is just the equatorial Podleś sphere [29]. The above quotients of $\mathscr{A}(SU_q(2))$ with respect to $\ker \pi_{\pm}$ either coincide with $\mathscr{A}(\mathbb{S}^2_q)$ or are quotients of it. Now, from (23) one sees that the spectrum of $\pi_{\pm}(b)$ is either real positive or real negative, depending on the $\pm$ sign. Hence, the algebras $\mathscr{A}(D^2_{q+})$ and $\mathscr{A}(D^2_{q-})$ describe the two hemispheres of $\mathbb{S}^2_q$ that are quantum disks.

A symbol map $\sigma : \mathscr{A}(D^2_{q\pm}) \to \mathscr{A}(\mathbb{S}^1)$ will map these "noncommutative disks" to their common boundary $\mathbb{S}^1$ which, as said, is the equator of the equatorial Podleś sphere $\mathbb{S}^2_q$. Explicitly, the map σ is the $*$-homomorphism given on the generators of $\mathscr{A}(D^2_{q,\pm})$ by

$$\sigma(r_{\pm}(a)) := u, \qquad \sigma(r_{\pm}(b)) := 0, \tag{25}$$

where u is the unitary generator of $\mathscr{A}(\mathbb{S}^1)$.

The following result emulates Proposition 4 of [9].

Proposition 21. *There is a $*$-homomorphism*

$$\rho : \mathscr{B} \to \mathscr{A}(D^2_{q+}) \otimes \mathscr{A}(D^2_{q-}) \otimes \mathscr{A}(\mathbb{S}^1) \tag{26}$$

defined on generators by

$$\rho(\tilde{a}_+) := r_+(a) \otimes r_-(a) \otimes u, \qquad \rho(\tilde{a}_-) := -q\, r_+(b) \otimes r_-(b^*) \otimes u^*,$$
$$\rho(\tilde{b}_+) := -r_+(a) \otimes r_-(b) \otimes u, \qquad \rho(\tilde{b}_-) := -r_+(b) \otimes r_-(a^*) \otimes u^*$$

while the off-diagonal operators $a_/$ and $b_/$ are declared to lie in the kernel of ρ.

Definition 22. The *cosphere bundle on $SU_q(2)$*, denoted by $\mathscr{A}(\mathbb{S}^*_q)$, is defined as the range of the map ρ in $\mathscr{A}(D^2_{q+}) \otimes A(D^2_{q-}) \otimes \mathscr{A}(\mathbb{S}^1)$.

Note that $\mathbb{S}^*_q$ coincides with the cosphere bundle defined in [9, 10], where it is regarded as a noncommutative space over which $D^2_{q+} \times D^2_{q-} \times \mathbb{S}^1$ is fibred.

We again follow [9] for the computation of the dimension spectrum. In order to do that, we define on the algebras $\mathscr{A}(D^2_{q\pm})$ three linear functionals τ_1 and $\tau_0^{\uparrow}$, $\tau_0^{\downarrow}$. Since their definitions for both disks D^2_{q+} and D^2_{q-} are identical, we shall omit the $\pm$ for notational convenience. For $x \in \mathscr{A}(D^2_q)$, and σ the symbol map (25), we define,

$$\tau_1(x) := \frac{1}{2\pi} \int_{S^1} \sigma(x),$$
$$\tau_0^{\uparrow}(x) := \lim_{N\to\infty} \mathrm{Tr}_N\, \pi(x) - \left(N + \frac{3}{2}\right)\tau_1(x),$$
$$\tau_0^{\downarrow}(x) := \lim_{N\to\infty} \mathrm{Tr}_N\, \pi(x) - \left(N + \frac{1}{2}\right)\tau_1(x),$$

where Tr_N is the truncated trace $\mathrm{Tr}_N(T) := \sum_{k=0}^{N} \langle \varepsilon_k | T \varepsilon_k \rangle$. The definition of the two different maps $\tau_0^{\uparrow}$ and $\tau_0^{\downarrow}$ is suggested by the constants $\frac{3}{2}$ and $\frac{1}{2}$ appearing in our choice (19) of the Dirac operator. Some simple algebra gives

$$\mathrm{Tr}_N(\pi(x)) = \left(N + \frac{3}{2}\right)\tau_1(x) + \tau_0^{\uparrow}(x) + O(N^{-k})$$
$$= \left(N + \frac{1}{2}\right)\tau_1(x) + \tau_0^{\downarrow}(x) + O(N^{-k}) \quad \text{for all } k > 0.$$

Let us use the notation of [12], defining the noncommutative integral as a zeta residue,

$$⨍\, T := \mathrm{Res}_{z=0}\, \mathrm{Tr}\, T|D|^{-z}.$$

Also, let us denote by r the restriction homomorphism from $\mathscr{A}(D^2_{q+}) \otimes A(D^2_{q-}) \otimes \mathscr{A}(\mathbb{S}^1)$ onto the first two legs of the tensor product. In particular, we will use it as a map

$$r : \mathscr{A}(\mathbb{S}^*_q) \to \mathscr{A}(D^2_{q+}) \otimes A(D^2_{q-}).$$

Theorem 23. *The dimension spectrum of the spectral triple* $(\mathscr{A}(SU_q(2)), \mathscr{H}, D)$ *is simple and given by* $\{1, 2, 3\}$. *With* $T \in \Psi^0(\mathscr{A})$, *the corresponding residues are*

$$\fint T|D|^{-3} = 2(\tau_1 \otimes \tau_1)\big(r\rho(T)^0\big),$$
$$\fint T|D|^{-2} = \big(\tau_1 \otimes (\tau_0^{\uparrow} + \tau_0^{\downarrow}) + (\tau_0^{\uparrow} + \tau_0^{\downarrow}) \otimes \tau_1\big)\big(r\rho(T)^0\big),$$
$$\fint T|D|^{-1} = (\tau_0^{\uparrow} \otimes \tau_0^{\downarrow} + \tau_0^{\downarrow} \otimes \tau_0^{\uparrow})\big(r\rho(T)^0\big).$$

Here $\rho(T)^0$ is the degree-zero part with respect to the $\mathbb{Z}$-grading on $\mathscr{A}(\mathbb{S}^*_q)$ induced (in its representation) by the one-parameter group of automorphisms $\gamma(t)$ generated by $|D|$:

$$\gamma(t) : T \mapsto e^{it|D|} T e^{-it|D|},$$

for any operator T on $\mathscr{H}$.

5.2 The Local Index Formula for 3-Dimensional Geometries

Let us recall that with any odd spectral triple $(\mathscr{A}, \mathscr{H}, D)$ there comes a Fredholm index of the operator D as an additive map $\varphi : K_1(\mathscr{A}) \to \mathbb{Z}$. If $F = \operatorname{Sign} D$ and P is the projector $P = \frac{1}{2}(1 + F)$ then, with $u \in \operatorname{Mat}_r(\mathscr{A})$ a unitary representative of the K_1 class, the operator PuP is automatically Fredholm and the index map is defined by,

$$\varphi([u]) := \operatorname{Index}(PuP) = \dim\ker PUP - \dim\ker PU^*P. \tag{27}$$

This map is computed by pairing $K_1(\mathscr{A})$ with "nonlocal" cyclic cocycles χ_n given in terms of the operator F and of the form

$$\chi_n(a_0, \ldots, \alpha_n) = \lambda_n \operatorname{Tr}(a_0 [F, a_1] \ldots [F, a_n]), \quad \text{for all } a_j \in \mathscr{A}, \tag{28}$$

where λ_n is a suitable normalization constant [7]. The choice of the integer n is determined by the degree of summability of the Fredholm module $(\mathscr{H}, F)$ over $\mathscr{A}$. Any such module is declared to be p-summable if the commutator $[F, a]$ is an element in the p-th Schatten ideal $\mathscr{L}^p(\mathscr{H})$, for any $a \in A$. The minimal n in (28) needs to be taken such that $n \geq p$.

On the other hand, the Connes–Moscovici local index theorem [12] expresses the index map in terms of a local cocycle φ_{odd} in the (b, B) bicomplex of $\mathscr{A}$, a cocycle which is a local representative of the cyclic cohomology class of χ_n (the cyclic cohomology Chern character). The cocycle φ_{odd} is given in terms of the operator D and is made of a finite number of terms $\varphi_{\text{odd}} = (\varphi_1, \varphi_3, \ldots)$; the pairing of the cyclic cohomology class $[\varphi_{\text{odd}}] \in HC^{\text{odd}}(\mathscr{A})$ with $K_1(\mathscr{A})$ gives the Fredholm index (27) of the operator D with coefficients in $K_1(\mathscr{A})$. Components of the cyclic cocycle φ_{odd} are explicitly given in [12], and we shall soon give them for our case.

We know from Theorem 12 that our spectral triple $(\mathscr{A}, \mathscr{H}, D)$ with $\mathscr{A} = \mathscr{A}(SU_q(2))$ has metric dimension 3. The corresponding Fredholm module $(\mathscr{H}, F)$ over $\mathscr{A} = \mathscr{A}(SU_q(2))$ is 1-summable since all commutators $[F, \pi(x)]$, with $x \in \mathscr{A}$, are off-diagonal operators given by sequences of rapid decay, thus each $[F, \pi(x)]$ is trace-class. Hence, we only need the first Chern character $\chi_1(a_0, a_1) = \mathrm{Tr}(a_0 [F, a_1])$, with $a_1, a_2 \in \mathscr{A}$. An explicit expression for this cyclic cocycle on the PBW-basis of $SU_q(2)$ was obtained in [25].

The local cocycle has two components, $\varphi_{\mathrm{odd}} = (\varphi_1, \varphi_3)$, with the cocycle condition $(b + B)\varphi_{\mathrm{odd}} = 0$ reading $B\varphi_1 = 0$, $b\varphi_1 + B\varphi_3 = 0$, $b\varphi_3 = 0$. It is explicitly given by

$$\varphi_1(a_0, a_1) := \fint a_0 [D, a_1] |D|^{-1} - \frac{1}{4} \fint a_0 \nabla([D, a_1]) |D|^{-3} + \frac{1}{8} \fint a_0 \nabla^2([D, a_1]) |D|^{-5},$$

$$\varphi_3(a_0, a_1, a_2, a_3) := \frac{1}{12} \fint a_0 [D, a_1][D, a_2][D, a_3] |D|^{-3},$$

where $\nabla(T) := [D^2, T]$ for any operator T on $\mathscr{H}$. Under the assumption that $[F, a]$ is traceclass for each $a \in \mathscr{A}$, these expressions can be rewritten as follows:

$$\varphi_1(a_0, a_1) = \fint a_0 \delta(a_1) F |D|^{-1} - \frac{1}{2} \fint a_0 \delta^2(a_1) F |D|^{-2} + \frac{1}{4} \fint a_0 \delta^3(a_1) F |D|^{-3},$$

$$\varphi_3(a_0, a_1, a_2, a_3) = \frac{1}{12} \fint a_0 \delta(a_1) \delta(a_2) \delta(a_3) F |D|^{-3}.$$

We now quote Proposition 2 of [9].

Proposition 24 (Connes). *Let $(\mathscr{A}, \mathscr{H}, D)$ be a spectral triple with discrete simple dimension spectrum not containing 0 and bounded above by 3. If $[F, a]$ is trace-class for all $a \in \mathscr{A}$, then the Chern character χ_1 is equal to $\varphi_{\mathrm{odd}} - (b + B)\varphi_{\mathrm{ev}}$ where the η-cochain $\varphi_{\mathrm{ev}} = (\varphi_0, \varphi_2)$ is given by*

$$\varphi_0(a) := \mathrm{Tr}(Fa |D|^{-z})\big|_{z=0},$$

$$\varphi_2(a_0, a_1, a_2) := \frac{1}{24} \fint a_0 \delta(a_1) \delta^2(a_2) F |D|^{-3}.$$

The definition of φ_0 needs the absence of 0 in the dimension spectrum. In components, the equivalence of the characters means that $\varphi_1 = \chi_1 + b\varphi_0 + B\varphi_2$ and $\varphi_3 = b\varphi_2$.

The above proposition, in combination with the following general result, shows that, up to coboundaries, the term χ_1 can be given by means of one single (b, B)-cocycle ψ_1.

Proposition 25. *Let $(\mathscr{A}, \mathscr{H}, D)$ be a spectral triple with discrete simple dimension spectrum not containing 0 and bounded above by 3. Assume that $[F, a]$ is trace class for all $a \in \mathscr{A}$, and set $P := \frac{1}{2}(1 + F)$. Then, the local Chern character φ_{odd} is equal to $\psi_1 - (b + B)\varphi'_{\text{ev}}$, where*

$$\psi_1(a_0, a_1) := 2 \int a_0\, \delta(a_1) P |D|^{-1} - \int a_0\, \delta^2(a_1) P |D|^{-2} + \frac{2}{3} \int a_0\, \delta^3(a_1) P |D|^{-3},$$

and $\varphi'_{\text{ev}} = (\varphi'_0, \varphi'_2)$ is given by

$$\varphi'_0(a) := \operatorname{Tr}(a\, |D|^{-z})\big|_{z=0},$$
$$\varphi'_2(a_0, a_1, a_2) := -\frac{1}{24} \int a_0\, \delta(a_1)\, \delta^2(a_2) F |D|^{-3}.$$

In the previous expression, the term involving $P|D|^{-3}$ would vanish if the latter were traceclass, which is the case in [9]. Combining these last two propositions, it follows that the cyclic 1-cocycles χ_1 and ψ_1 are related as

$$\chi_1 = \psi_1 - b\beta, \quad \text{where } \beta(a) = 2 \operatorname{Tr}(Pa\, |D|^{-z})\big|_{z=0}. \tag{29}$$

5.3 The Pairing Between HC^1 and K_1

As an example, we shall compute the value of the index map (27) when U is the unitary operator representing the generator of $K_1(\mathscr{A}(SU_q(2)))$,

$$U = \begin{pmatrix} a & b \\ -qb^* & a^* \end{pmatrix}, \tag{30}$$

acting on the doubled Hilbert space $\mathscr{H} \otimes \mathbb{C}^2$ via the representation $\pi \otimes 1_2$. One expects this index to be nonzero, since the K-homology class of $(\mathscr{A}, \mathscr{H}, D)$ is non-trivial.

We first compute directly the above index. Remember that the projector P was earlier denoted $P^{\uparrow}$. A short computation shows that the kernel of PU^*P is trivial, whereas the kernel of PUP contains only elements proportional to the vector

$$\begin{pmatrix} |0, 0, -\frac{1}{2}, \uparrow\rangle \\ -q^{-1}|0, 0, \frac{1}{2}, \uparrow\rangle \end{pmatrix},$$

leading to $\varphi([U]) = \text{Index}(PUP) = 1$.

Our Fredholm module $(\mathscr{H}, F)$ over $\mathscr{A}(SU_q(2))$ is 1-summable; and we have just seen that $\text{Index}(PUP)$ can be computed using the local cyclic cocycle ψ_1 in (29). To prepare for this index computation via ψ_1, we recall the following lemma [7, IV.1.γ], which fixes the normalization constant in front of χ_1.

Lemma 26 (Connes). *Let $(\mathscr{H}, F)$ be a 1-summable Fredholm module over $\mathscr{A}$, with projector $P = \frac{1}{2}(1+F)$; and let $u \in \mathrm{Mat}_r(\mathscr{A})$ be unitary with a suitable r. Then PuP is a Fredholm operator on $P\mathscr{H}$ and*

$$\mathrm{Index}(PuP) = -\frac{1}{2}\,\mathrm{Tr}(u^*[F,u]) = -\frac{1}{2}\chi_1(u^*,u).$$

Thus, the index of PUP, for the U of (30) is given, up to an overall $-\frac{1}{2}$ factor, by

$$\begin{aligned}&\psi_1(U^{-1},U)\\ &\quad = 2\int U_{kl}^*\,\delta(U_{lk})P|D|^{-1} - \int U_{kl}^*\,\delta^2(U_{lk})P|D|^{-2} + \frac{2}{3}\int U_{kl}^*\,\delta^3(U_{lk})P|D|^{-3},\end{aligned}$$

with summation over $k,l = 0,1$ understood. Since the entries of U are generators of $\mathscr{A}(SU_q(2))$, we see from (20b) for a and its analogue for b that $\rho(\delta^2(U_{kl})) = \rho(U_{kl})$. We compute the degree 0 part of $\rho(U_{kl}^*\,\delta(U_{lk}))$ with respect to the grading coming from $\gamma(t)$, which is the only part that contributes to the trace, using the algebra relations of $\mathscr{A}(D^2_{q\pm})$,

$$\rho(U_{kl}^*\,\delta(U_{lk}))^0 = 2(1-q^2)\,1\otimes r_-(b)^2.$$

Using the equalities

$$\tau_1(1) = 1, \qquad \tau_1(r_\pm(b)^n) = 0,$$

and

$$\tau_0^{\uparrow}(1) = -\tau_0^{\downarrow}(1) = -\frac{1}{2}, \qquad \tau_0^{\uparrow}(r_\pm(b)^n) = \tau_0^{\downarrow}(r_\pm(b)^n) = \frac{(\pm 1)^n}{1-q^n},$$

we find that

$$\begin{aligned}&\psi_1(U^{-1},U)\\ &\quad = 2(1-q^2)(2\tau_0^{\uparrow}\otimes\tau_0^{\downarrow} + \tfrac{2}{3}\tau_1\otimes\tau_1)(1\otimes r_-(b)^2)\\ &\qquad - (\tau_1\otimes\tau_0^{\downarrow} + \tau_0^{\uparrow}\otimes\tau_1)(1\otimes 1) = -2.\end{aligned}$$

Taking the proper coefficients, we finally obtain

$$\mathrm{Index}(PUP) = -\frac{1}{2}\psi_1(U^{-1},U) = 1.$$

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Topological Strings on Local Curves

Marcos Mariño

Abstract We review some perturbative and nonperturbative aspects of topological string theory on the Calabi–Yau manifolds $X_p = \mathscr{O}(-p) \oplus \mathscr{O}(p-2) \to \mathbb{P}^1$. These are exactly solvable models of topological string theory which exhibit a nontrivial yet simple phase structure, and have a phase transition in the universality class of pure two-dimensional gravity. They don't have conventional mirror description, but a mirror B model can be formulated in terms of recursion relations on a spectral curve typical of matrix model theory. This makes it possible to calculate nonperturbative, spacetime instanton effects in a reliable way, and in particular to characterize the large order behavior of string perturbation theory.

1 Introduction

Topological string theory on non-compact Calabi–Yau manifolds (also known as local Calabi–Yau's) has taught us many interesting things about topological strings and about string theory in general. Although non-compact backgrounds are quite special, their relative simplicity makes them also a fascinating laboratory. From the mathematical point of view, the theory of topological strings on local backgrounds has made a myriad of connections to other fields of mathematics and mathematical physics, including matrix models, integrable systems, and combinatorics.

Among these local backgrounds, perhaps the simplest and the most peculiar are what I will call *local curves*. This is the family of non-compact Calabi–Yau manifolds given by the total space of a bundle over a sphere. More concretely, they have the form

$$X_p = \mathscr{O}(p-2) \oplus \mathscr{O}(-p) \to \mathbb{P}^1, \quad p \in \mathbb{Z}. \tag{1}$$

Marcos Mariño
Département de Physique Théorique and Section de Mathématiques, Université de Genève, 1211 Genève 4, Switzerland, e-mail: marcos.marino@unige.ch

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This family includes two of the most studied local backgrounds: for $p = 1$ one recovers the resolved conifold, while X_2 is the $\mathbb{C} \times A_1$ singularity. Therefore, the family (1) provides the simplest generalization of these well studied examples.

The study of topological string theory on X_p has led to many insights. For example, the conjecture relating toric backgrounds to matrix models stated in [26] and further refined in [5] was motivated to a large extent by the genus zero solution on X_p presented in [8]. These backgrounds have been an important testing ground for recent techniques and ideas, but one has to keep in mind that they are rather unconventional in many respects.

In this note we review some properties of topological string theory on X_p discovered in [8, 26, 27]. We summarize them briefly in this introduction by emphasizing both their connections to general aspects of topological string theory, as well as their idiosyncrasies.

- *A-model and topological vertex*. The Gromov–Witten theory for these spaces was developed by Bryan and Pandharipande [6] and can be reproduced, in the equivariant case, by the topological vertex of [1]. The total partition sum in the A model is a sum over partitions. This is reviewed in Sect. 2.1.
- *Sum over partitions and mirror symmetry*. The backgrounds X_p do not have standard mirror manifolds (see however [17, 18] for some progress along this direction). However, a mirror geometry can be extracted by studying the saddle-point of the sum over partitions [8] and it is encoded in a complex curve which we will call the spectral curve of the model. This is similar to the way in which the Seiberg–Witten curve emerges from the sum over partitions in Nekrasov's computation [28, 29]. The mirror geometry is reviewed in Sect. 2.3
- *Matrix models*. The generating functionals of Gromov–Witten invariants at genus g, F_g, can be obtained by applying the matrix model formalism of [16] to the spectral, mirror curve. This was conjectured and tested to lower genus in [26]. Therefore, topological strings on X_p can be described by a matrix model formalism. The matrix model/topological string correspondence was first found by [13] in some special affine backgrounds and later generalized to toric manifolds [26, 5]. In the case of X_p the existence of a matrix model description was proved by Eynard in [15]. This development is briefly mentioned in Sect. 2.4
- *Phase transitions*. As for other topological string models, the free energies F_g of X_p exhibit singular behavior for $p > 2$ at a particular point $t_c \neq 0$ in the Kähler moduli space. For most topological string models, this point is the conifold point and the singular behavior is described by the $c = 1$ string at self-dual radius [19]. In the case of topological string theory on local curves, however, the singular behavior is described by the $c = 0$ string, i.e. by two-dimensional gravity [8]. Phase transitions on X_p are described in Sect. 3.
- *Instantons and large order behavior*. The matrix model formalism makes possible to compute spacetime instanton corrections to the partition function [27]. Using the connection between instantons and large order behavior, one obtains conjectural, precise descriptions of the asymptotic behavior of the couplings F_g at large g [26, 27] which can be tested numerically. This aspect is reviewed in Sect. 4.

- *Hurwitz theory*. In the limit $p \to \infty$, topological strings on local curves encode the simple Hurwitz numbers of $\mathbb{P}^1$. This is established in Sect. 2.2. Most of the properties above can be seen to be inherited by this Hurwitz model (like in particular the critical behavior and the instanton effects describing large order), and we refer for this to the original papers [8, 27].

We finally mention that the study of these backgrounds was originally motivated by the results of [2] and the connection to the OSV conjecture [30].

2 Topological Strings on Local Curves

First, we notice that since X_p is invariant under $-p \leftrightarrow p-2$ we can restrict ourselves to the case $p > 0$.

2.1 A Model

The first step in understanding topological string theory on X_p is to determine the genus g free energies of closed strings in the A model. Already this is nontrivial, since as explained in [6], the A model has to be defined equivariantly with respect to an action of $\mathbb{C}^* \times \mathbb{C}^*$ on the bundles. Therefore, the most general topological string theory on X_p will depend on two equivariant parameters s_1, s_2. The most natural choice (also called the equivariant Calabi–Yau case) corresponds to the antidiagonal action, in which $s_1 = -s_2$. It can be shown that in this case the dependence on the equivariant parameters drops out, and one obtains topological closed string amplitudes $F_g(t)$ which only depend on the Kähler parameter t (corresponding to the $\mathbb{P}^1$ in the base). We recall that, when expanded around $t = \infty$, the $F_g(t)$ are generating functionals of Gromov–Witten invariants at genus g,

$$F_g(t) = \sum_{k=1}^{\infty} N_{g,k} \mathrm{e}^{-kt}, \tag{2}$$

where k corresponds to the degree of the map. As usual in topological string theory, the $F_g(t)$ are put together into a single total free energy,

$$F_{X_p}(g_s, t) = \sum_{g=0}^{\infty} g_s^{2g-2} F_g^{X_p}(t) \tag{3}$$

and its exponential is the closed partition function

$$Z_{X_p} = \exp F_{X_p}(g_s, t). \tag{4}$$

This partition function was computed in [6] and we can equivalently calculate it by using the theory of the topological vertex [1]. We collect here some formulae from this theory will be useful in the following. First of all, we define the q-number $[n]$ as

$$[n] = q^{n/2} - q^{-n/2}, \qquad q = \mathrm{e}^{g_s}. \tag{5}$$

A representation R of $U(\infty)$ is encoded by a Young tableau, labeled by the lengths of its rows $\{l_i\}$. The quantity

$$\ell(R) = \sum_i l_i \tag{6}$$

is the total number of boxes of the tableau. Another important quantity associated to a tableau is

$$\kappa_R = \sum_i l_i(l_i - 2i + 1). \tag{7}$$

We also introduce the quantity

$$W_R = q^{-\kappa_R/4} \prod_{\square \in R} \frac{1}{[\mathrm{hook}(\square)]}. \tag{8}$$

We can now write the topological string partition function on X_p. It is given in terms of the W_R by

$$Z_{X_p} = \sum_R W_R W_{R^t} q^{(p-1)\kappa_R/2} Q^{\ell(R)}, \quad Q = (-1)^p \mathrm{e}^{-t}. \tag{9}$$

Although (9) gives an all-genus expression, it is effectively an expansion in powers of Q. One can easily compute the first few terms in the expansion:

$$\begin{aligned} F_0^{X_p}(t) &= (-1)^p \mathrm{e}^{-t} + \frac{1}{8}(2p^2 - 4p + 1)\mathrm{e}^{-2t} \\ &\quad + \frac{(-1)^p}{54}(1 - 6p + 3p^2)(2 - 6p + 3p^2)\mathrm{e}^{-3t} + \mathscr{O}(\mathrm{e}^{-4t}), \\ F_1^{X_p}(t) &= -\frac{(-1)^p}{12}\mathrm{e}^{-t} + \frac{1}{48}(p^4 - 4p^3 + p^2 + 6p - 2)\mathrm{e}^{-2t} \\ &\quad + \frac{(-1)^p}{72}(-2 + 14p - 19p^2 - 20p^3 + 45p^4 - 24p^5 + 4p^6)\mathrm{e}^{-3t} \\ &\quad + \mathscr{O}(\mathrm{e}^{-4t}), \end{aligned} \tag{10}$$

and so on.

2.2 Relation to Hurwitz Theory

The partition function Z_{X_p} can be regarded as a "quantum deformation" of a simpler theory, namely the counting of simple Hurwitz covers of $\mathbb{P}^1$. To see this, we first note

that the quantity W_R is a q-deformation of the dimension d_R of the representation R of $S_{\ell(R)}$, the permutation group of $\ell(R)$ elements: as $g_s \to 0$, one has that

$$W_R \to g_s^{-\ell(R)} \frac{d_R}{|\ell(R)|!}. \tag{11}$$

This suggests taking the following limit,

$$g_s \to 0, \quad t \to \infty, \quad p \to \infty, \tag{12}$$

in such a way that

$$pg_s = \tau_2/N, \quad (-1)^p \mathrm{e}^{-t} = (g_s N)^2 \mathrm{e}^{-\tau_1}, \tag{13}$$

and τ_1, τ_2 and N are new parameters that are kept fixed. In the limit (12)–(13) the partition function becomes

$$Z_{X_p} \to Z_{\text{Hurwitz}} = \sum_R \left(\frac{d_R}{|\ell(R)|!} \right)^2 N^{2\ell(R)} \mathrm{e}^{-\tau_2 \kappa_R/2N} \mathrm{e}^{-\tau_1 \ell(R)}. \tag{14}$$

This is the generating functional of simple Hurwitz numbers of $\mathbb{P}^1$ at all genus and degrees. Recall that Hurwitz theory studies branched covers of Riemann surfaces, and Hurwitz numbers enumerate these coverings for fixed genus and degree. When all branch points are simple, the Hurwitz number is called a *simple Hurwitz number*, and for $\mathbb{P}^1$ it is given at genus g and degree d by

$$H^{\mathbb{P}^1}_{g,d}(1^d) = \sum_{\ell(R)=d} \left(\frac{d_R}{\ell(R)!} \right)^2 (\kappa_R/2)^{2g-2+2d}, \tag{15}$$

where the sum is over representations R with fixed number of boxes equal to the degree d. Using this formula we can rewrite (14) as

$$\begin{aligned} Z_{\text{Hurwitz}} &= \sum_{d,m} N^{2d-m} \mathrm{e}^{-\tau_1 d} \sum_{\ell(R)=d} \left(\frac{d_R}{\ell(R)!} \right)^2 \frac{(-\tau_2)^m}{m!} (\kappa_R/2)^m \\ &= \sum_{g \geq 0} N^{2-2g} \sum_{d \geq 0} \mathrm{e}^{-\tau_1 d} H^{\mathbb{P}^1}_{g,d}(1^d) \frac{\tau_2^{2g-2+2d}}{(2g-2+2d)!}, \end{aligned} \tag{16}$$

where in the second line we have traded the sum over m by a sum over g. Notice that, since $\kappa_{R^t} = -\kappa_R$, only even powers of τ_2 appear. The model described by (14) has been studied in detail due to its connection to Hurwitz theory. From the physical point of view, it was analyzed in [23, 9], and in the mathematical literature it has been studied for example in [20].

The free energy of Z_{Hurwitz} describes *connected*, simple Hurwitz numbers $H^{\mathbb{P}^1}_{g,d}(1^d)^\bullet$:

$$F_{\text{Hurwitz}} = \log Z_{\text{Hurwitz}} = \sum_{g\geq 0} N^{2-2g} \sum_{d\geq 0} \mathrm{e}^{-\tau_1 d} H^{\mathbb{P}^1}_{g,d}(1^d)^\bullet \frac{\tau_2^{2g-2+2d}}{(2g-2+2d)!} \quad (17)$$

If we compare this to the total free energy F_{X_p} written in (3) in terms of Gromov–Witten invariants, and take the limit (12)–(13), we find

$$\lim_{p\to\infty} p^{2-2g-2d}(-1)^p N_{g,d}(p) = \frac{H^{\mathbb{P}^1}_{g,d}(1^d)^\bullet}{(2g-2+2d)!}. \quad (18)$$

The l.h.s. is precisely the coefficient of the highest power in p of $N_{g,d}(p)$. We can therefore interpret the Gromov–Witten invariants of this model as q–deformed connected, simple Hurwitz numbers, since they promote $H^{\mathbb{P}^1}_{g,d}(1^d)^\bullet$ to polynomials of degree $2g-2+2d$ (which is equal to the number of simple branch points).

2.3 Mirror Symmetry from Large Partitions

Sums over partitions of the form (9) are sometimes dominated by a single Young tableau which can be regarded as the "saddle point" of the sum over partitions. This approach has been very useful in understanding for example two-dimensional Yang–Mills theory [14] or Nekrasov's instanton sums [29]. Moreover, one expects that, if the total partition function Z_{X_p} can be described by mirror symmetry, the mirror geometry will be encoded in the saddle point of the sum over partitions (this is for example the case in instanton sums, whose mirror description is the special geometry of the Seiberg–Witten curves). Since we don't have an easy way to construct the mirror geometry, we will *deduce it* as a saddle partition of the sum (9). We summarize now the results of this deduction, first performed in [8].

The first step is to notice that (9) admits a representation in terms of a q-deformed group theoretical quantity of $U(N)$, similarly to what was done in [23] in a similar context. Let $\{l_i\}$ be the lengths of rows in a Young tableau introduced before, and let $h_i = l_i + N - i$. We can write

$$Z_{X_p} = \sum_R \left(\frac{\dim_q R}{{}_q\Omega_R}\right)^2 q^{(p-1)\kappa_R/2} \mathrm{e}^{-t\ell(R)} \quad (19)$$

where

$${}_q\Omega_R = \prod_{i=1}^N \frac{[h_i]!}{[N-i]!}, \quad (20)$$

and

$$\dim_q R = \prod_{1\leq i<j\leq N} \frac{[l_i - l_j + j - i]}{[j-i]} \quad (21)$$

is the quantum dimension of an irreducible representation R of $U(N)$. If we introduce the auxiliary 't Hooft parameter

$$T = g_s N \tag{22}$$

and continuous variables in the standard way:

$$\frac{h_i}{N} = \frac{l_i}{N} - \frac{i}{N} + 1 \to \ell(x) - x + 1 = h(x), \tag{23}$$

we find that at large N the sum over partitions is controlled by an effective action for continuous variables

$$\begin{aligned} S = &- \int_0^1 \int_0^1 \mathrm{d}x\mathrm{d}y \log\left|2\sinh\frac{T}{2}(h(x) - h(y))\right| + \frac{2}{T}\int_0^1 \mathrm{d}x \mathrm{Li}_2(\mathrm{e}^{-Th}) \\ &+ \int_0^1 dx h(x)(t - (p-1)T) \\ &+ \frac{pT}{2}\int_0^1 \mathrm{d}x h^2(x) + (p-1)\frac{T}{3} - \frac{\pi^2}{3T} - \frac{1}{2}t. \end{aligned} \tag{24}$$

The planar limit is governed by a tableau density

$$\rho(h) = -\frac{\mathrm{d}x(h)}{\mathrm{d}h}, \tag{25}$$

which one can find as the saddle-point of the effective action. The result is the following.

It is useful to introduce the variable

$$\lambda = \exp\bigl(1 - hT\bigr). \tag{26}$$

In terms of this variable, the density of tableaux $\rho(\lambda)$ has its support on the interval

$$(x_2, x_1) \cup (x_1, \mathrm{e}), \tag{27}$$

where $x_{1,2}$ are nontrivial functions of the Kähler parameter t. To specify these, one introduces the *mirror map*

$$Q = (-1)^p \mathrm{e}^{-t} = (1-\zeta)^{-p(p-2)}\zeta. \tag{28}$$

The endpoints of the cut are given in terms of ζ by

$$x_1 = (1-\zeta)^{-p}(1+\zeta^{\frac{1}{2}})^2, \quad x_2 = (1-\zeta)^{-p}(1-\zeta^{\frac{1}{2}})^2. \tag{29}$$

The information on $\rho(\lambda)$ is equivalently encoded in the resolvent

$$\omega_0(\lambda) = \int_{x_2}^{\mathrm{e}} \frac{\mathrm{d}v}{v}\,\frac{\rho(v)}{\lambda - v} - \frac{1}{\lambda}\log\frac{\lambda}{\lambda - \mathrm{e}}, \tag{30}$$

which according to [8] is given by

$$\omega_0(\lambda) = \frac{1}{\lambda} + \frac{p}{2\lambda} \log\left[2\frac{\sqrt{(\lambda - x_1)(\lambda - x_2)} - \lambda - \sqrt{x_1 x_2}}{(\sqrt{x_1} + \sqrt{x_2})^2} \right]^2 + \frac{1}{\lambda} \log\left[\frac{(\sqrt{\lambda - x_1} + \sqrt{\lambda - x_2})^2}{4\lambda} \right]. \tag{31}$$

This function has a branch cut along $[x_1, x_2]$, and its discontinuity is given by

$$y(\lambda) = \frac{2}{\lambda}\left(\tanh^{-1}\left[\frac{\sqrt{(\lambda - x_1)(\lambda - x_2)}}{\lambda - \frac{x_1 + x_2}{2}} \right] - p \tanh^{-1}\left[\frac{\sqrt{(\lambda - x_1)(\lambda - x_2)}}{\lambda + \sqrt{x_1 x_2}} \right] \right). \tag{32}$$

It is well known that the mirrors to toric Calabi–Yau threefolds can be reduced to algebraic curves. In [26] it was proposed that $y = y(\lambda)$ is the appropriate mirror curve for the X_p geometry. This can be tested in various ways, and we will review some of them below. We then have a mirror geometry obtained from a saddle-point analysis of a sum over tableaux.

This analysis makes possible to compute the genus zero free energy in closed form. As detailed in [8], one finds that

$$\frac{\mathrm{d}^2 F_0}{\mathrm{d}t^2} = -\log(1 - \zeta). \tag{33}$$

We can also provide a closed expansion for the prepotential F_0 as a series in e^{-t}. This is better done by working out the expansion of $\log(1 - \zeta)$ through Lagrange inversion and integrating (33) twice. In this way we obtain

$$F_0^{X_p}(t) = \sum_{d=1}^{\infty} \frac{1}{d!} \frac{1}{d^2} \frac{((p-1)^2 d - 1)!}{(((p-1)^2 - 1)d)!} (-1)^{dt} \mathrm{e}^{-dt}. \tag{34}$$

2.4 Higher Genus and Matrix Models

It was conjectured in [26] that the higher F_g of this model can be obtained by using the matrix model formalism of [16] as applied to the mirror curve (31). This conjecture was later proved by Eynard [15] by providing an explicit matrix integral representation of Z_{X_p}. For example, using this formalism one finds that

$$F_1 = -\frac{1}{24} \log\left[\frac{(p-1)^2 \zeta(\zeta_c - \zeta)}{(1 - \zeta)^3} \right]. \tag{35}$$

This genus one amplitude can be written as

$$F_1 = F_1^{\mathrm{inst}} + \frac{1}{24} \log\, Q, \tag{36}$$

where F_1^{inst} is the instanton part of F_1 which follows from (9).

3 Phase Transitions, Critical Behavior and Double-Scaling Limit

3.1 Review of Phase Transitions in Topological String Theory

For simplicity, we will assume in this general discussion that the Calabi–Yau X has a single Kähler parameter t, i.e. $h^{1,1}(X) = 1$ (this is in fact the case for the case we are studying, X_p). When t is large (in the so-called large radius regime) the geometry probed by string theory can be regarded as a classical geometry together with stringy corrections. This is well reflected in the structure of the prepotential $F_0(t)$ or genus zero topological string amplitude, which in the large radius regime is of the form

$$F_0(t) = \frac{C}{6}t^3 + \sum_{k=1}^{\infty} N_{0,k}\mathrm{e}^{-kt}. \tag{37}$$

In this equation, C is the classical intersection number for the two-cycle whose size is measured by t. The infinite sum in the r.h.s. is given by worldsheet instanton corrections, which are obtained by "counting" (in an appropriate sense) holomorphic maps from $\mathbb{P}^1$ to X. The instanton counting numbers $N_{0,k}$ are genus zero Gromov–Witten invariants, and we have chosen units in which $\ell_s = \sqrt{2\pi}$.

The series of worldsheet instanton corrections, regarded as a power series in e^{-t}, has in general a finite radius of convergence t_c which can be obtained by looking at the asymptotic growth with k of the numbers $N_{0,k}$. We will characterize this asymptotic growth by t_c and by a critical exponent γ:

$$N_{0,k} \sim k^{\gamma-3}\mathrm{e}^{kt_c}, \quad k \to \infty. \tag{38}$$

When this holds, the prepotential behaves near t_c as

$$F_0(t) \sim (\mathrm{e}^{-t_c} - \mathrm{e}^{-t})^{2-\gamma}. \tag{39}$$

It turns out that typical Gromov–Witten invariants of Calabi–Yau manifolds behave asymptotically as

$$N_{0,k} \sim \frac{\mathrm{e}^{kt_c}}{k^3 \log^2 k}, \quad k \to \infty. \tag{40}$$

This is of the form (38), with critical exponent

$$\gamma = 0 \tag{41}$$

and subleading log corrections. This behavior was first established in [7] in the example of the quintic, and since then it has been verified in other examples, like for example in local $\mathbb{P}^2$, where the critical radius is given by [3, 22]

$$t_c = \frac{1}{\Gamma(\frac{1}{3})\Gamma(\frac{2}{3})}\mathrm{Re}\, G\left(\frac{1}{3}, \frac{2}{3}, 1; 1\right) \sim 2.90759 \tag{42}$$

and G is the Meijer function.

The subleading log in (40) leads to log corrections near the critical point (also referred to as scaling violations) of the form

$$F_0(t) \sim (\mathrm{e}^{-t_c} - \mathrm{e}^{-t})^2 \log(\mathrm{e}^{-t_c} - \mathrm{e}^{-t}). \tag{43}$$

This is the genus zero free energy of the $c = 1$ string at the self–dual radius, once the scaling variable $\mathrm{e}^{-t_c} - \mathrm{e}^{-t}$ is identified with the cosmological constant [4, 19].

The behavior of the prepotential gives a precise quantitative meaning to the distinction between classical and quantum geometry. We will refer to the divergence of the large radius expansion at $t = t_c$ as a *phase transition* with a critical exponent γ defined in (40). The phase with

$$t > t_c \tag{44}$$

where the expansion (37) is convergent, is called the large radius or Calabi–Yau phase, where classical geometry makes sense (albeit it is corrected by worldsheet instantons). When $t \leq t_c$, the nonlinear sigma model approach is not well defined, and classical geometric intuition is misleading.

In order to describe the phase structure of the model we have relied on the behavior of the prepotential, i.e. the planar free energy. It is natural to ask what happens when higher genus topological string amplitudes are taken into account. It turns out that the higher genus Gromov–Witten invariants have the asymptotic behavior [4]

$$N_{g,k} \sim k^{(\gamma-2)(1-g)-1} \mathrm{e}^{kt_c}, \quad k \to \infty, \tag{45}$$

where t_c is the critical radius obtained at genus zero and it is common to all g, and γ is the critical exponent that appears in (38). This is equivalent to the following behavior near the critical point

$$\begin{aligned} F_1(t) &\sim c_1 \log(\mathrm{e}^{-t_c} - \mathrm{e}^{-t}), \\ F_g(t) &\sim c_g (\mathrm{e}^{-t_c} - \mathrm{e}^{-t})^{(1-g)(2-\gamma)}, \quad g \geq 2. \end{aligned} \tag{46}$$

In conventional topological string theory, as we have mentioned, $\gamma = 0$, but the more general form we have written above will be useful later.

We then see that the phase transition at $t = t_c$ is common for all $F_g(t)$, and the critical exponent changes with the genus in the way prescribed by (45). This sort of coherent behavior in the genus expansion is not obvious, but seems to characterize a wide variety of systems that admit a genus expansion (like for example matrix models, see [12] for a review). When this is the case, one can define a *double-scaling limit* as follows. Let us consider the total free energy F as a perturbative expansion in powers of the string coupling constant g_s:

$$F(g_s, t) = \sum_{g=0}^{\infty} F_g(t) g_s^{2g-2}. \tag{47}$$

We define the double-scaled string coupling as

$$\kappa = a g_s (\mathrm{e}^{-t_c} - \mathrm{e}^{-t})^{\gamma/2-1}, \tag{48}$$

where a is an appropriate constant. We can then consider the limit

$$t \to t_c, \qquad g_s \to 0, \qquad \kappa \text{ fixed}. \tag{49}$$

In this limit, only the most singular part of $F_g(t)$ survives at each genus, and the total free energy becomes the *double-scaled free energy*

$$F_{\mathrm{ds}}(\kappa) = f_0 \kappa^{-2} + f_1 \log \kappa + \sum_{g \geq 2} f_g \kappa^{2g-2}, \tag{50}$$

where $f_g = a^{2-2g} c_g$. It is also customary to express the double-scaled free energy in terms of the scaling variable $z = \kappa^{2/(\gamma-2)}$.

It turns out that, in some cases, one can determine the coefficients f_g in closed form. In the double-scaling limit of matrix models, they are governed by a differential equation of the Painlevé type [12]. In the case of topological string theory on Calabi–Yau manifolds, it was conjectured in [19] that, in terms of a natural coordinate

$$\mu \sim \mathrm{e}^{-t_c} - \mathrm{e}^{-t} \tag{51}$$

which in the mirror model measures the distance to the conifold point $\mu = 0$, the double-scaled free energy is universal and reads

$$F_{\mathrm{ds}}(\mu) = \frac{1}{2}\mu^2 \log \mu - \frac{1}{12} \log \mu + \sum_{g=2}^{\infty} \frac{B_{2g}}{2g(2g-2)} \mu^{2-2g}. \tag{52}$$

This is exactly the all genus free energy of the $c = 1$ string at the self-dual radius. This behavior has been checked in many examples (see, for example, [21] for a recent calculation on the quintic Calabi–Yau).

3.2 Phase Transitions for Local Curves

Surprisingly, the theory of local curves displays a phase transition, but in a different universality class than the usual topological strings on Calabi–Yau threefolds. As shown in [8], the phase transition of local curves belong to the universality class of 2d gravity.

The easiest way to see this is to analyze the asymptotic growth of genus zero Gromov–Witten invariants. We found in (34),

$$N_{0,k} = \frac{1}{k! k^2} \frac{((p-1)^2 k - 1)!}{(((p-1)^2 - 1)k)!}, \tag{53}$$

up to a sign $(-1)^{pk}$. By using Stirling's formula, we obtain

$$N_{0,k} \sim \mathrm{e}^{kt_c} k^{-7/2}, \quad k \to \infty, \tag{54}$$

where

$$t_c = \log\big((p(p-2))^{p(2-p)}(p-1)^{2(p-1)^2}\big). \tag{55}$$

This corresponds to

$$\zeta_c = \frac{1}{(p-1)^2}, \tag{56}$$

By comparing to (38) we also deduce that

$$\gamma = -\frac{1}{2}. \tag{57}$$

The above results are valid for $p > 2$. For $p = 1, 2$ the series is convergent for all $t > 0$. The above result for the critical exponent γ is *not* the standard one for Calabi–Yau threefolds, and indicates that we are in a different universality class.

What is this universality class? (57) is the exponent typical of 2d gravity (see for example [12] for a review and references), and in fact, if one takes the double-scaling limit

$$\zeta \to \zeta_c, \quad g_s \to 0, \quad z \text{ fixed}, \tag{58}$$

where

$$z^{5/2} = g_s^{-2} \frac{(p-1)^8}{4(1-\zeta_c)^3}(\zeta_c - \zeta)^5, \tag{59}$$

then the total free energy (3) becomes the free energy of 2d gravity,

$$F_{(2,3)}(z) = -\frac{4}{15} z^{5/2} - \frac{1}{48} \log z + \sum_{g \geq 2} a_g z^{-5(g-1)/2}, \tag{60}$$

where the coefficients a_g can be obtained by solving the Painlevé I equation

$$u^2 - \frac{1}{6} u'' = z \tag{61}$$

satisfied by the specific heat

$$u(z) = -F''_{(2,3)}(z). \tag{62}$$

Evidence for this result was given in [8]. One can test it at lower genus for all p, and for all genera in the limit $p \to \infty$ (i.e. Hurwitz theory) by using for example [20]. In fact, this result follows from the description of this theory in terms of a matrix model conjectured in [26] and proved in [15]. It follows from [16] that the computation of symplectic invariants F_g of a given spectral curve commutes with the double-scaling limit. Therefore, it is enough to show that the curve (32) becomes the spectral curve characterizing 2d gravity. Let us verify this.

We first notice that near the critical point the endpoints of the curve behave as

$$x_1 = x_1^{(c)} + \theta(\zeta - \zeta_c) + \mathscr{O}(\zeta - \zeta_c)^2, \qquad x_2 = x_2^{(c)} + \mathscr{O}(\zeta - \zeta_c)^2 \tag{63}$$

where

$$\begin{aligned} x_1^{(c)} &= (1-\zeta_c)^{-p}\frac{p^2}{(p-1)^2}, \\ x_2^{(c)} &= (1-\zeta_c)^{-p}\frac{(p-2)^2}{(p-1)^2}, \\ \theta &= 2(1-\zeta_c)^{-p}\frac{p(p-1)}{p-2}. \end{aligned} \tag{64}$$

The coordinate λ in (32) must scale in this limit like

$$\lambda = x_1^{(c)} - \theta(\zeta - \zeta_c)s + \mathscr{O}(\zeta - \zeta_c)^2. \tag{65}$$

This defines the "renormalized" coordinate s. We now reexpress (32) in terms of the scaling variables s and z, which is given in (59). After some cancellations, we find that

$$\frac{1}{g_s}y(\lambda)\mathrm{d}\lambda \to y(s)\mathrm{d}s = -\frac{4\sqrt{2}}{3}z^{\frac{5}{4}}(2s-1)\sqrt{1+s}\,\mathrm{d}s, \tag{66}$$

for all $p > 2$. This is the spectral curve of the $(2, 3)$ model, therefore we have proved our claim. We can also interpret the r.h.s. as the Laplace transform of the macroscopic loop operator of 2d gravity, which corresponds to the disk amplitude of the FZZT brane of Liouville theory (see [25] and references therein).

4 Non-perturbative Effects and Large Order Behavior

It was pointed out in [26] that the matrix model description of this topological string models can be used to describe spacetime instantons. In matrix models, instanton effects are associated to eigenvalue tunneling [31, 10, 11], and in fact it is possible to write down explicit formulae for the instanton amplitudes up to two loops by using only information from the spectral curve [27].

Let us describe the instanton amplitudes for a matrix model described by a curve of the form

$$y(z) = M(z)\sqrt{(z-x_1)(z-x_2)}, \tag{67}$$

The saddle points where the eigenvalues tunnel are located at

$$M(x_0) = 0. \tag{68}$$

The instanton action for an instanton tunneling to x_0 is simply given by

$$A = \int_{x_1}^{x_0} y(p)\mathrm{d}p. \tag{69}$$

There might be many possible saddles x_0, and as usual the leading contribution comes from the instanton with larger action (in absolute value). The one-loop fluctuation around the instanton is given by

$$\mu = -\mathrm{i}\,\frac{x_1 - x_2}{4}\sqrt{\frac{1}{2\pi M'(x_0)[(x_0 - x_2)(x_0 - x_1)]^{\frac{5}{2}}}}. \tag{70}$$

The instanton action and one-loop fluctuation are in general complex,

$$A = |A|\mathrm{e}^{\mathrm{i}\theta_A}, \qquad \mu = |\mu|\mathrm{e}^{\mathrm{i}\theta_\mu}. \tag{71}$$

Using the standard connection between instantons and large order behaviour (see for example [24]) one finds that the F_g behave at large g as

$$F_g \sim \frac{|A|^{-2g-b}}{\pi}\,\Gamma(2g+b)\,|\mu|\,\cos\bigl((2g+b)\theta_A + \theta_\mu\bigr). \tag{72}$$

where in the case of one-cut Hermitian matrix models and topological strings on local curves [27]

$$b = -\frac{5}{2}. \tag{73}$$

As we explained in Sect. 2, the F_g amplitudes of topological string theory on local curves can be computed by the matrix model formalism of [16] applied to the curve (32), as discussed in [26]. Therefore, we can apply the general expressions above to compute instanton amplitudes in terms of spectral curve data, and we can indeed verify that the large order of the F_g is governed by (72). In order to apply formulae (69), (70) we have to find the location of the saddle x_0 in (68). For the cases $p = 3$ and $p = 4$ the relevant solutions have been determined in [26]; they are given by

$$x_0 = \frac{4x_1x_2}{(\sqrt{x_1} - \sqrt{x_2})^2}, \qquad p = 3, \tag{74}$$

and

$$x_0 = \frac{2\sqrt{x_1}x_2}{\sqrt{x_1} - \sqrt{x_2}}, \qquad p = 4. \tag{75}$$

An explicit expression for the instanton action was also computed in [26]; it is given by the expression

$$A(Q) = F(x_0) - F(x_1), \tag{76}$$

where

$$
\begin{aligned}
F(x) = &-\log(f_1(x))\left(\log(f_1(x)) - 2\log\left(1+\frac{2f_1(x)}{(\sqrt{x_1}-\sqrt{x_2})^2}\right)\right.\\
&\left.+\log\left(1+\frac{2f_1(x)}{(\sqrt{x_1}+\sqrt{x_2})^2}\right)\right) - 2\mathrm{Li}_2\left(-\frac{2f_1(x)}{(\sqrt{x_1}-\sqrt{x_2})^2}\right)\\
&-2\mathrm{Li}_2\left(-\frac{2f_1(x)}{(\sqrt{x_1}+\sqrt{x_2})^2}\right) - \log\frac{(x_1-x_2)^2}{4}\log x\\
&-p\log(f_2(x))\left(\log(f_2(x)) + 2\log\left(1-\frac{f_2(x)}{2\sqrt{x_1x_2}}\right)\right.\\
&\left.-\log\left(1-\frac{2f_2(x)}{(\sqrt{x_1}+\sqrt{x_2})^2}\right)\right) - 2p\mathrm{Li}_2\left(-\frac{f_2(x)}{2\sqrt{x_1x_2}}\right)\\
&+2p\mathrm{Li}_2\left(\frac{2f_2(x)}{(\sqrt{x_1}+\sqrt{x_2})^2}\right)\\
&+\frac{p}{2}(\log x)^2 + p\log(\sqrt{x_1}+\sqrt{x_2})^2\log x, \qquad (77)
\end{aligned}
$$

and

$$
\begin{aligned}
f_1(x) &= \sqrt{(x-x_1)(x-x_2)} + x - \frac{x_1+x_2}{2},\\
f_2(x) &= \sqrt{(x-x_1)(x-x_2)} + x + \sqrt{x_1x_2}.
\end{aligned} \qquad (78)
$$

We can now numerically compare the behavior of the sequence F_g with the instanton prediction (72). Since we have only computed ten terms in the sequence F_g, we need standard acceleration methods to extract the asymptotics with some precision. For example, assuming (72) holds, we can extract numerically the value of A and compare to the instanton prediction. In order to extract A, we consider the sequence

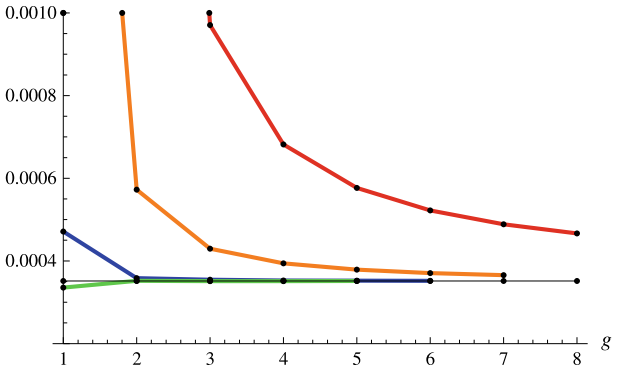

Fig. 1 The sequence S_g and the first three Richardson transforms for the local curve X_3, at the fixed value $\zeta = 0.24$. The leading asymptotics are predicted to be given by the instanton action $A(\zeta)$, shown as a straight line. The error for the available degree $g = 8$ is 0.014%

$$S_g = 2g\sqrt{\frac{F_g}{F_{g+1}}} = A + \mathcal{O}(1/g) \tag{79}$$

for a fixed value of ζ, and its Richardson transforms $S_g^{(N)}$ for $N = 1, 2, \ldots$, which help to eliminate the subleading tail $\mathcal{O}(1/g)$. The resulting sequences $S_g^{(N)}(\zeta)$ should converge to $A(\zeta)$, therefore they define numerical approximations to $A(\zeta)$. In Fig. 1 we show, for $p = 3$, the sequence S_g at $\zeta = 0.24$ and its Richardson transforms for $N = 1, 2, 3$. The instanton prediction for A is the straight line. As we can see, the agreement between the numerical extrapolation and the instanton prediction is remarkable.

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Repeated Interaction Quantum Systems

Marco Merkli

Abstract We consider a quantum system interacting sequentially with elements of a chain of independent quantum subsystems. We treat two kinds of such repeated interaction systems: deterministic and random ones. In both cases we show that, under suitable conditions, the system approaches an asymptotic state in the large time limit, and we construct that state.

Our methods are based on the analysis of products of operators generating the dynamics at each step in the process of repeated interaction. In the random case, we obtain results about infinite products of independent, identically distributed random matrices.

1 Introduction

Consider a quantum system $\mathscr{S}$ which interacts with another one, $\mathscr{E}_1$, during a time interval $[0, \tau_1)$, then for times $[\tau_1, \tau_1 + \tau_2)$, $\mathscr{S}$ interacts with another system $\mathscr{E}_2$, and so on. The assembly of the $\mathscr{E}_k$, which we suppose to be independent of each other (i.e., not directly coupled), is called a chain, $\mathscr{C} = \mathscr{E}_1 + \mathscr{E}_2 + \cdots$. The system $\mathscr{S} + \mathscr{C}$ is called a *repeated interaction quantum system*. One may think of $\mathscr{S}$ as being the system of interest, say a particle enclosed in a container, and of $\mathscr{C}$ as a chain of measuring apparatuses $\mathscr{E}_k$ that are brought into contact with the particle in a sequential manner. The system $\mathscr{S}$ is an *open quantum system*, which is coupled to the "environment" $\mathscr{C}$. Our goal to study the influence of the chain on $\mathscr{S}$, and to describe the (asymptotic) dynamics of the latter system.

The theoretical and practical importance of repeated interaction quantum systems is exemplified by systems of radiation-matter coupling, where atoms interact with modes of the quantized electromagnetic field. In this setting, the system $\mathscr{S}$

Marco Merkli
Department of Mathematics and Statistics, Memorial University of Newfoundland, St. John's, NL A1C 5S7, Canada, e-mail: merkli@mun.ca

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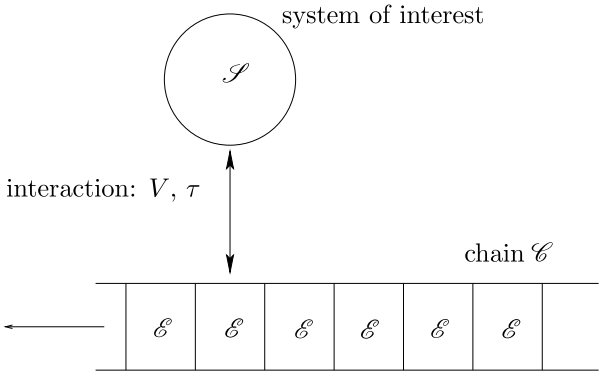

Fig. 1 A repeated interaction system

describes one or several modes of the field in a cavity and the chain $\mathscr{C}$ represents a beam of atoms $\mathscr{E}$ injected into the cavity. So-called "One-Atom Masers", where the beam is tuned in such a way that at each given moment a *single atom* is inside a microwave cavity and the interaction time τ is the same for each single atom, have been experimentally realized in laboratories [10, 11]. After interaction, the atoms encode certain properties of the field that can be measured after they exit the cavity.

We distinguish two classes of models of repeated interaction quantum systems. In *deterministic models*, each system $\mathscr{E}_k$ is the a copy of a single quantum system $\mathscr{E}$, and the interactions between $\mathscr{S}$ and $\mathscr{C}$ are determined by a fixed interaction time $\tau > 0$ and interaction operator V (acting on $\mathscr{S}$ and $\mathscr{E}$), τ, V being independent of the interaction step. While deterministic models are interesting quantum dynamical systems in their own right, it is clear that they are idealized mathematical models, if supposed to describe physical experiments (as for instance the "One-Atom Maser"). Indeed, in actual experiments, neither the way of interaction, nor the interaction time, nor the elements $\mathscr{E}$ will be exactly the same for each step in the process. Rather, the interaction time should be considered to be *random*, for instance given by a Gaussian (or a uniform) distribution around a mean value. Further, the atoms in experiments are ejected from an atom oven, then they are cooled down to a wanted temperature before entering the cavity. Of course one cannot have absolute control over their preparation or their interaction with the field in the cavity. Thus the state of the incoming atoms should also be taken random, for instance determined by a temperature that fluctuates slightly around a mean temperature. It is therefore important to develop a theory that allows for *random repeated interaction systems*, which is the second class of systems we consider. The randomness may have different sources, it may come from fluctuations in the incoming elements $\mathscr{E}_k$, or in the interaction, via random interaction times τ_k and/or random interaction operators V.

Literature

The reader will find in [4, 5] a more detailed list of related works. Mathematical work on systems similar to the ones considered here is done in [12], using entirely different methods. The part of our work dealing with products of random matrices and random ergodic theorems is linked to many other works, see the references in [5].

2 Deterministic Systems

It is more convenient for the reader to first consider deterministic models, and to pass to random ones in a second step. We describe our systems within the framework of algebraic quantum statistical mechanics. An introduction to this can be found e.g. in [2, 3].

2.1 Mathematical Description

The deterministic models consist of a system $\mathscr{S}$ which is coupled to a chain $\mathscr{C} = \mathscr{E} + \mathscr{E} + \cdots$ of identical elements $\mathscr{E}$. We describe $\mathscr{S}$ and $\mathscr{E}$ as W^*-dynamical systems $(\mathfrak{M}_{\mathscr{S}}, \alpha^t_{\mathscr{S}})$ and $(\mathfrak{M}_{\mathscr{E}}, \alpha^t_{\mathscr{E}})$, where $\mathfrak{M}_{\mathscr{S}}$, $\mathfrak{M}_{\mathscr{E}}$ are von Neumann algebras "of observables" acting on the Hilbert spaces $\mathscr{H}_{\mathscr{S}}$, $\mathscr{H}_{\mathscr{E}}$, respectively, and where $\alpha^t_{\mathscr{S}}$ and $\alpha^t_{\mathscr{E}}$ are (σ-weakly continuous) groups of $*$automorphisms describing the Heisenberg dynamics. In this paper, we consider the situation $\dim \mathscr{H}_{\mathscr{S}} < \infty$ and $\dim \mathscr{H}_{\mathscr{E}} \leq \infty$.

We assume that there are distinguished *reference vectors* $\psi_{\mathscr{S}} \in \mathscr{H}_{\mathscr{S}}$ and $\psi_{\mathscr{E}} \in \mathscr{H}_{\mathscr{E}}$, determining states on $\mathfrak{M}_{\mathscr{S}}$ and $\mathfrak{M}_{\mathscr{E}}$ which are invariant w.r.t. $\alpha^t_{\mathscr{S}}$ and $\alpha^t_{\mathscr{E}}$, respectively, and we assume that $\psi_{\mathscr{S}}$ and $\psi_{\mathscr{E}}$ are cyclic and separating for $\mathfrak{M}_{\mathscr{S}}$ and $\mathfrak{M}_{\mathscr{E}}$, respectively. One may take equilibrium (KMS) vectors for these reference vectors.

The Hilbert space of the chain $\mathscr{C}$ is defined to be the infinite tensor product

$$\mathscr{H}_{\mathscr{C}} = \otimes_{m \geq 1} \mathscr{H}_{\mathscr{E}} \tag{1}$$

w.r.t. the reference vector

$$\psi_{\mathscr{C}} = \psi_{\mathscr{E}} \otimes \psi_{\mathscr{E}} \cdots . \tag{2}$$

In other words, $\mathscr{H}_{\mathscr{C}}$ is obtained by taking the completion of the vector space of finite linear combinations of the form $\otimes_{m \geq 1} \phi_m$, where $\phi_m \in \mathscr{H}_{\mathscr{E}}$, $\phi_m = \psi_{\mathscr{E}}$ except for finitely many indices, in the norm induced by the inner product

$$\langle \otimes_m \phi_m, \otimes_m \chi_m \rangle = \prod_m \langle \phi_m, \chi_m \rangle_{\mathscr{H}_{\mathscr{E}}} . \tag{3}$$

We introduce the von Neumann algebra

$$\mathfrak{M}_{\mathscr{C}} = \otimes_{m\geq 1}\mathfrak{M}_{\mathscr{E}} \tag{4}$$

acting on $\otimes_{m\geq 1}\mathscr{H}_{\mathscr{E}}$, which is obtained by taking the weak closure of finite linear combinations of operators $\otimes_{m\geq 1}A_m$, where $A_m \in \mathfrak{M}_{\mathscr{E}}$ and $A_m = \mathbb{1}_{\mathscr{H}_{\mathscr{E}}}$ except for finitely many indices.

The operator algebra containing the observables of the total system is the von Neumann algebra

$$\mathfrak{M} = \mathfrak{M}_{\mathscr{S}} \otimes \mathfrak{M}_{\mathscr{C}} \tag{5}$$

which acts on the Hilbert space

$$\mathscr{H} = \mathscr{H}_{\mathscr{S}} \otimes \mathscr{H}_{\mathscr{C}}. \tag{6}$$

The *repeated interaction dynamics* of observables in $\mathfrak{M}$ is characterized by an interaction time $0 < \tau < \infty$ and a selfadjoint interaction operator

$$V \in \mathfrak{M}_{\mathscr{S}} \otimes \mathfrak{M}_{\mathscr{E}}. \tag{7}$$

For times $t \in [\tau(m-1), \tau m)$, where $m \geq 1$, $\mathscr{S}$ interacts with the m-th element of the chain, while all other elements of the chain evolve freely (each one according to the dynamics $\alpha_{\mathscr{E}}$). The interaction of $\mathscr{S}$ with every element in the chain is the same (given by V).

Let $L_{\mathscr{S}}$ and $L_{\mathscr{E}}$ be the *standard Liouville operators* ("positive temperature Hamiltonians", cf. references of [7, 9]), uniquely characterized by the following properties: $L_{\#}$ (where $\# = \mathscr{S}, \mathscr{E}$) are selfadjoint operators on $\mathscr{H}_{\#}$ which implement the dynamics $\alpha^t_{\#}$,

$$\alpha^t_{\#}(A) = \mathrm{e}^{\mathrm{i}tL_{\#}} A \mathrm{e}^{-\mathrm{i}tL_{\#}}, \quad \forall A \in \mathfrak{M}_{\#},\ \forall t \in \mathbb{R} \tag{8}$$

and satisfy

$$L_{\#}\psi_{\#} = 0. \tag{9}$$

We define the selfadjoint operator

$$L = L_{\mathscr{S}} + L_{\mathscr{E}} + V, \tag{10}$$

omitting trivial factors $\mathbb{1}_{\mathscr{S}}$ or $\mathbb{1}_{\mathscr{E}}$ (by $L_{\mathscr{S}}$ in (10) we really mean $L_{\mathscr{S}} \otimes \mathbb{1}_{\mathscr{E}}$, etc). L generates the group of $*$automorphisms $\mathrm{e}^{\mathrm{i}tL} \cdot \mathrm{e}^{-\mathrm{i}tL}$ of $\mathfrak{M}_{\mathscr{S}} \otimes \mathfrak{M}_{\mathscr{E}}$, the interacting dynamics between $\mathscr{S}$ and an element $\mathscr{E}$ of the chain $\mathscr{C}$. The explicit form of the operator V is dictated by the underlying physics, we give some examples in Sect. 4.

For $m \geq 1$ let us denote by

$$\widetilde{L}_m = L_m + \sum_{k\neq m} L_{\mathscr{E},k} \tag{11}$$

the generator of the total dynamics during the interval $[(m-1)\tau, m\tau)$. We have introduced L_m, the operator on $\mathscr{H}$ that acts trivially on all elements of the chain except for the m-th one. On the remaining part of the space (which is isomorphic to $\mathscr{H}_{\mathscr{S}} \otimes \mathscr{H}_{\mathscr{E}}$), L_m acts as L, (10). We have also set $L_{\mathscr{E},k}$ to be the operator on $\mathscr{H}$ that acts nontrivially only on the k-th element of the chain, on which it equals $L_{\mathscr{E}}$. Of course, the infinite sum in (11) must be interpreted in the strong sense on $\mathscr{H}$.

Decompose $t \in \mathbb{R}_+$ as

$$t = m(t)\tau + s(t), \tag{12}$$

where $m(t)$ is the integer measuring the number of complete interactions of duration τ the system $\mathscr{S}$ has undergone at time t, and where $0 \leq s(t) < \tau$. The repeated interaction dynamics of an operator A on $\mathscr{H}$ is defined by

$$\alpha^t_{\mathrm{RI}}(A) = U_{\mathrm{RI}}(t)^* A U_{\mathrm{RI}}(t), \tag{13}$$

where the unitary

$$U_{\mathrm{RI}}(t) = \mathrm{e}^{-\mathrm{i}s(t)\widetilde{L}_{m(t)+1}} \mathrm{e}^{-\mathrm{i}\tau\widetilde{L}_{m(t)}} \cdots \mathrm{e}^{-\mathrm{i}\tau\widetilde{L}_1} \tag{14}$$

defines the Schrödinger dynamics on $\mathscr{H}$. According to this dynamics, $\mathscr{S}$ interacts in succession, for a fixed duration τ and a fixed interaction V, with the first $m(t)$ elements of the chain, and for the remaining duration $s(t)$ with the $(m(t)+1)$-th element of the chain.

Our goal is to examine the large time behaviour of expectation values of certain observables in normal states ϱ on $\mathfrak{M}$ (states given by a density matrix on $\mathscr{H}$). The system $\mathscr{S}$ feels an *effective dynamics* induced by the interaction with the chain $\mathscr{C}$. Under a suitable *ergodicity assumption* on this effective dynamics the small system is driven to an asymptotic state, as time increases. We will express the effective dynamics and the ergodic assumption using the modular data of the pair $(\mathfrak{M}_{\mathscr{S}} \otimes \mathfrak{M}_{\mathscr{C}}, \psi_{\mathscr{S}} \otimes \psi_{\mathscr{C}})$.

Let J and Δ denote the modular conjugation and the modular operator associated to $(\mathfrak{M}_{\mathscr{S}} \otimes \mathfrak{M}_{\mathscr{E}}, \psi_{\mathscr{S}} \otimes \psi_{\mathscr{E}})$, [3]. We assume that

(A) $\Delta^{1/2} V \Delta^{-1/2} \in \mathfrak{M}_{\mathscr{S}} \otimes \mathfrak{M}_{\mathscr{E}}$

and we introduce the operator

$$K = L - J\Delta^{1/2} V \Delta^{-1/2} J, \tag{15}$$

called the Liouville operator associated to $\psi_{\mathscr{S}} \otimes \psi_{\mathscr{E}}$, [7, 9]. It generates a strongly continuous group of bounded operators, denoted $\mathrm{e}^{\mathrm{i}tK}$, satisfying

$$\|\mathrm{e}^{\mathrm{i}tK}\| \leq \mathrm{e}^{|t|\,\|\Delta^{1/2} V \Delta^{-1/2}\|}.$$

The main feature of the operator K is that $\mathrm{e}^{\mathrm{i}tK}$ implements the same dynamics as $\mathrm{e}^{\mathrm{i}tL}$ on $\mathfrak{M}_{\mathscr{S}} \otimes \mathfrak{M}_{\mathscr{E}}$ (since the difference $K - L$ belongs to the commutant $\mathfrak{M}'_{\mathscr{S}} \otimes \mathfrak{M}'_{\mathscr{E}}$), and that

$$K\psi_{\mathscr{S}} \otimes \psi_{\mathscr{E}} = 0. \tag{16}$$

Relation (16) follows from assumption (A), definition (15) and the properties

$$\Delta^{-1/2} J = J\Delta^{1/2} \quad \text{and} \quad J\Delta^{1/2} A\psi_{\mathscr{S}} \otimes \psi_{\mathscr{E}} = A^*\psi_{\mathscr{S}} \otimes \psi_{\mathscr{E}},$$

for any $A \in \mathfrak{M}_{\mathscr{S}} \otimes \mathfrak{M}_{\mathscr{E}}$.

Let

$$P = \mathbb{1}_{\mathscr{H}_{\mathscr{S}}} \otimes |\psi_{\mathscr{C}}\rangle\langle\psi_{\mathscr{C}}| \tag{17}$$

be the orthogonal projection onto $\mathscr{H}_{\mathscr{S}} \otimes \mathbb{C}\psi_{\mathscr{C}} \cong \mathscr{H}_{\mathscr{S}}$, where $\psi_{\mathscr{C}}$ is given in (2). Given an operator B on $\mathscr{H}$, we identify PBP with an operator acting on $\mathscr{H}_{\mathscr{S}}$. We have

Proposition 1 ([4]). *There is a constant $C < \infty$ s.t. $\|(P\mathrm{e}^{\mathrm{i}tK}P)^m\|_{\mathscr{B}(\mathscr{H}_{\mathscr{S}})} \leq C$, for all $t \in \mathbb{R}$, $m \geq 0$. In particular,* $\mathrm{spec}(P\mathrm{e}^{\mathrm{i}tK}P) \subset \{z \in \mathbb{C} \mid |z| \leq 1\}$, *and all eigenvalues lying on the unit circle are semisimple.*

Relation (16) implies $P\mathrm{e}^{\mathrm{i}tK}P\psi_{\mathscr{S}} = \psi_{\mathscr{S}}$, for all $t \in \mathbb{R}$. Our assumption (E) on the effectiveness of the coupling is an ergodicity assumption on the discrete dynamics generated by

$$M \equiv M(\tau) = P\mathrm{e}^{\mathrm{i}\tau K}P. \tag{18}$$

(E) The spectrum of M on the complex unit circle consists of the single eigenvalue $\{1\}$. This eigenvalue is simple (with corresponding eigenvector $\psi_{\mathscr{S}}$).

Assumption (E) guarantees that the adjoint operator M^* has a unique invariant vector, called $\psi^*_{\mathscr{S}}$ (normalized as $\langle\psi^*_{\mathscr{S}}, \psi_{\mathscr{S}}\rangle = 1$), and that

$$\lim_{m\to\infty} M^m = \pi := |\psi_{\mathscr{S}}\rangle\langle\psi^*_{\mathscr{S}}|, \tag{19}$$

in the operator sense, where π is the rank one projection which projects onto $\mathbb{C}\psi_{\mathscr{S}}$ along $(\mathbb{C}\psi^*_{\mathscr{S}})^{\perp}$. In fact, we have the following easy estimate (valid for any matrix M with spectrum inside the unit disk and satisfying (E)).

Proposition 2 ([4]). *For any $\epsilon > 0$ there exists a constant C_ϵ s.t. $\|M^m - \pi\| \leq C_\epsilon \mathrm{e}^{-m(\gamma-\epsilon)}$, for all $m \geq 0$, where $\gamma := \min_{z\in\mathrm{spec}(M)\setminus\{1\}} |\log|z|| > 0$.*

The parameter γ measures the speed of convergence. If all eigenvalues of M are semisimple, then we have, in Proposition 2, $\|M^m - \pi\| \leq C\mathrm{e}^{-m\gamma}$ for some constant C and all $m \geq 0$.

As a last preparation towards an understanding of our results we discuss the kinds of observables we consider. One interesting such class is $\mathfrak{M}_{\mathscr{S}} \subset \mathfrak{M}$ which consists of observables of the system $\mathscr{S}$ only. There are other observables of interest. We may think of the system $\mathscr{S}$ as being fixed in space and of the chain as passing by $\mathscr{S}$ so that at the moment t, the $(m(t)+1)$-th element $\mathscr{E}$ is located near $\mathscr{S}$, cf. (12). A detector placed in the vicinity of $\mathscr{S}$ can measure at this moment in time observables of $\mathscr{S}$ and those of the $(m(t)+1)$-th element in the chain, i.e., an

"instantaneous observable" of the form $A_{\mathscr{S}} \otimes \vartheta_{m(t)+1}(A_{\mathscr{E}})$, where $A_{\mathscr{S}} \in \mathfrak{M}_{\mathscr{S}}$, $A_{\mathscr{E}} \in \mathfrak{M}_{\mathscr{E}}$, and $\vartheta_m : \mathfrak{M}_{\mathscr{E}} \to \mathfrak{M}_{\mathscr{C}}$ is defined by

$$\vartheta_m(A_{\mathscr{E}}) = \mathbb{1}_{\mathscr{E}} \cdots \mathbb{1}_{\mathscr{E}} \otimes A_{\mathscr{E}} \otimes \mathbb{1}_{\mathscr{E}} \cdots \tag{20}$$

the $A_{\mathscr{E}}$ on the right side of (20) acting on the m-th factor in the chain. An example of such an observable is the energy flux (variation) of the system $\mathscr{S}$. We call the operator $A_{\mathscr{S}} \otimes \vartheta_{m+1}(A_{\mathscr{E}})$ an instantaneous observable determined by $A_{\mathscr{S}} \in \mathfrak{M}_{\mathscr{S}}$ and $A_{\mathscr{E}} \in \mathfrak{M}_{\mathscr{E}}$. One may consider more general observables, [4].

2.2 Results

Throughout this section we assume that Conditions (A) and (E) of the previous section are satisfied.

2.3 Asymptotic State

We consider the large time limit of expectations of instantaneous observables,

$$E(t) = \varrho\big(\alpha_{\mathrm{RI}}^t(A_{\mathscr{S}} \otimes \vartheta_{m(t)+1}(A_{\mathscr{E}}))\big), \tag{21}$$

for normal initial states ϱ on $\mathfrak{M}$. Define the state ϱ_+ on $\mathfrak{M}_{\mathscr{S}}$ by

$$\varrho_+(A_{\mathscr{S}}) = \big\langle \psi_{\mathscr{S}}^*, A_{\mathscr{S}} \psi_{\mathscr{S}} \big\rangle, \tag{22}$$

where $\psi_{\mathscr{S}}^*$ is defined before (19).

Theorem 3 ([4]). *Suppose that conditions* (A) *and* (E) *are satisfied, and let ϱ be a fixed normal state on $\mathfrak{M}$. For any $\epsilon > 0$ there is a constant C_ϵ s.t. for all $t \geq 0$*

$$|E(t) - E_+(t)| \leq C_\epsilon \, \mathrm{e}^{-t(\gamma-\epsilon)/\tau}, \tag{23}$$

where $\gamma > 0$ is given in Proposition 2, and where E_+ is the τ-periodic function

$$E_+(t) = \varrho_+\Big(P\alpha_{\mathrm{RI}}^{s(t)}\Big(A_{\mathscr{S}} \otimes A_{\mathscr{E}}\Big)P\Big). \tag{24}$$

Remarks. (1) Using (23) and the uniqueness of the limit, one can see that the state ϱ_+ does *not* depend on the choice of the reference state ψ_S.

(2) C_ϵ in Theorem 3 is uniform in τ for $\tau > 0$ varying in compact sets, and it is uniform in $\big\{A_{\mathscr{S}} \in \mathfrak{M}_{\mathscr{S}}, A_{\mathscr{E}} \subset \mathfrak{M}_{\mathscr{E}} \;\big|\; \|A_{\mathscr{S}}\| \, \|A_{\mathscr{E}}\| \leq \text{const.}\big\}$.

(3) We refer to [4] for corresponding results for more general variables.

2.4 Correlations & Reconstruction of Initial State

As Theorems 3 shows, the limit expectation values $E_+(t)$ are independent of the initial state (since the state ϱ_+ is, cf. (22)). However, limiting correlations are not, and their knowledge allows to reconstruct the initial state.

Fix a normal initial state ϱ on $\mathfrak{M}$ and let $A \in \mathfrak{M}$, $A_{\mathscr{S}} \in \mathfrak{M}_{\mathscr{S}}$, $A_{\mathscr{E}} \in \mathfrak{M}_{\mathscr{E}}$. We define the correlation between A and the instantaneous observable $A_{\mathscr{S}} \otimes \vartheta_{m(t)+1}(A_{\mathscr{E}})$ by

$$\mathscr{C}(t; A, A_{\mathscr{S}}, A_{\mathscr{E}}) = \varrho\big(A\, \alpha^t_{\mathrm{RI}}\big(A_{\mathscr{S}} \otimes \vartheta_{m(t)+1}(A_{\mathscr{E}})\big)\big). \tag{25}$$

Theorem 4 ([4]). *For any $\epsilon > 0$ there is a constant C_ϵ s.t. for all $t \geq 0$*

$$|\mathscr{C}(t; A, A_{\mathscr{S}}, A_{\mathscr{E}}) - \mathscr{C}_+(t; A, A_{\mathscr{S}}, A_{\mathscr{E}})| \leq C_\epsilon \mathrm{e}^{-t(\gamma-\epsilon)/\tau}, \tag{26}$$

where γ is given in Proposition 2, and where $\mathscr{C}_+$ is the τ-periodic limit correlation function

$$\mathscr{C}_+(t; A, A_{\mathscr{S}}, A_{\mathscr{E}}) = \varrho(A)\, \varrho_+\big(P\alpha^{s(t)}_{\mathrm{RI}}(A_{\mathscr{S}} \otimes A_{\mathscr{E}})P\big), \tag{27}$$

with ϱ_+ defined in (22).

Relation (27) shows that the initial state ϱ can be recovered from the knowledge of the asymptotic correlations $\mathscr{C}_+$ and the asymptotic state ϱ_+.

3 Random Systems

3.1 Dynamics and Random Matrix Products

We consider $\mathscr{S}$ to interact with a chain $\mathscr{C} = \mathscr{E}_1 + \mathscr{E}_2 + \cdots$, where the elements $\mathscr{E}_k$ may vary with k. Correspondingly, we have Hilbert spaces $\mathscr{H}_{\mathscr{S}}$, $\mathscr{H}_{\mathscr{E}_k}$, $\dim \mathscr{H}_{\mathscr{S}} < \infty$, $\dim \mathscr{H}_{\mathscr{E}_k} \leq \infty$ and von Neumann algebras of observables $\mathfrak{M}_{\mathscr{S}} \subset \mathscr{B}(\mathscr{H}_{\mathscr{S}})$, $\mathfrak{M}_{\mathscr{E}_k} \subset \mathscr{B}(\mathscr{H}_{\mathscr{E}_k})$, describing $\mathscr{S}$ and $\mathscr{E}_k$, respectively. The uncoupled dynamics are given by groups of $*$automorphisms, $\alpha^t_{\mathscr{S}}$, $\alpha^t_{\mathscr{E}_k}$ of $\mathfrak{M}_{\mathscr{S}}$, $\mathfrak{M}_{\mathscr{E}_k}$. We introduce, as in the deterministic case, *reference states* $\psi_{\mathscr{S}} \in \mathscr{H}_{\mathscr{S}}$ and $\psi_{\mathscr{E}_k} \in \mathscr{H}_{\mathscr{E}_k}$, which are cyclic and separating vectors for the corresponding von Neumann algebras. Typical choices are KMS states with respect to the uncoupled dynamics, at given temperatures. The total Hilbert space is $\mathscr{H} = \mathscr{H}_{\mathscr{S}} \otimes \mathscr{H}_{\mathscr{C}}$, where $\mathscr{H}_{\mathscr{C}} = \otimes_{k\geq 1}\mathscr{H}_{\mathscr{E}_k}$, where the infinite tensor product is taken with respect to the vector $\psi_0 = \psi_{\mathscr{S}} \otimes \psi_{\mathscr{C}}$, with $\psi_{\mathscr{C}} = \psi_{\mathscr{E}_1} \otimes \psi_{\mathscr{E}_2} \otimes \cdots$. The free dynamics is $\alpha^t_{\mathscr{S}} \otimes_{k\geq 1} \alpha^t_{\mathscr{E}_k}$, a group of $*$automorphisms on the von Neumann algebra $\mathfrak{M} = \mathfrak{M}_{\mathscr{S}} \otimes_{k\geq 1} \mathfrak{M}_{\mathscr{E}_k}$.

The interaction times are now given by $\tau_1, \tau_2, \ldots$, and the interaction operators by $V_k \in \mathfrak{M}_{\mathscr{S}} \otimes \mathfrak{M}_{\mathscr{E}_k}$. As in the deterministic case, there are self-adjoint Liouville operators $L_\#$, satisfying

$$\mathrm{e}^{\mathrm{i}tL_\#} A_\# \mathrm{e}^{-\mathrm{i}tL_\#} = \alpha^t_\#(A_\#), \quad \text{and} \quad L_\#\psi_\# = 0,$$

for all $t \in \mathbb{R}$, $A_\# \in \mathfrak{M}_\#$, where $\# = \mathscr{S}, \mathscr{E}_k$. We define the (discrete) repeated interaction Schrödinger dynamics of a state vector $\phi \in \mathscr{H}$, for $m \geq 0$, by

$$U(m)\phi = \mathrm{e}^{-\mathrm{i}\widetilde{L}_m} \cdots \mathrm{e}^{-\mathrm{i}\widetilde{L}_2} \mathrm{e}^{-\mathrm{i}\widetilde{L}_1} \phi,$$

where

$$\widetilde{L}_k = \tau_k L_k + \tau_k \sum_{n \neq k} L_{\mathscr{E}_n} \tag{28}$$

describes the dynamics during the time interval $[\tau_1 + \cdots + \tau_{k-1}, \tau_1 + \cdots + \tau_k)$, which corresponds to the time-step k of our discrete process. Here,

$$L_k = L_\mathscr{S} + L_{\mathscr{E}_k} + V_k, \tag{29}$$

acting on $\mathscr{H}_\mathscr{S} \otimes \mathscr{H}_{\mathscr{E}_k}$. Of course, we understand that the operator $L_{\mathscr{E}_n}$ in (28) acts nontrivially only on the n-th factor of the Hilbert space $\mathscr{H}_\mathscr{E}$ of the chain.

Our goal is to understand the large-time asymptotics ($m \to \infty$) of expectations

$$\varrho(U(m)^* O U(m)) = \varrho(\alpha_{\mathrm{RI}}^m(O)), \tag{30}$$

for normal states ϱ and instantaneous observables O. We denote the repeated interaction dynamics in this setting by

$$\alpha_{\mathrm{RI}}^m(O) = U(m)^* O U(m). \tag{31}$$

Next, as in the deterministic case, we introduce new generators of the dynamics. Let J_m and Δ_m denote the modular data of the pair $(\mathfrak{M}_\mathscr{S} \otimes \mathfrak{M}_{\mathscr{E}_m}, \psi_\mathscr{S} \otimes \psi_{\mathscr{E}_m})$ (see e.g. [3]). In analogy with condition (A) (before (15)), we suppose that

(A′) $\Delta_m^{1/2} V_m \Delta_m^{-1/2} \in \mathfrak{M}_\mathscr{S} \otimes \mathfrak{M}_{\mathscr{E}_m}$, $\forall m \geq 1$.

Let us define the Liouville operator K_m, compare with (15), by

$$K_m = \tau_m \big[L_\mathscr{S} + L_{\mathscr{E}_m} + V_m - J_m \Delta_m^{1/2} V_m \Delta_m^{-1/2} J_m \big]. \tag{32}$$

Its main dynamical features,

$$\mathrm{e}^{\mathrm{i}\tau_m L_m} A \mathrm{e}^{-\mathrm{i}\tau_m L_m} = \mathrm{e}^{\mathrm{i}K_m} A \mathrm{e}^{-\mathrm{i}K_m}, \quad \text{for } A \in \mathfrak{M}_\mathscr{S} \otimes \mathfrak{M}_\mathscr{E}, \tag{33}$$

$$K_m \psi_\mathscr{S} \otimes \psi_{\mathscr{E}_m} = 0, \tag{34}$$

(see also (16)), are proven to hold by using standard relations of the modular data Δ_m, J_m, see e.g. [4]. Note also the bound $\|\mathrm{e}^{\pm i K_m}\| \leq \mathrm{e}^{\tau_m \|\Delta_m^{1/2} V_m \Delta_m^{-1/2}\|}$.

Denote by $P = \mathbb{1}_\mathscr{S} \otimes P_\mathscr{E}$ the projection onto the subspace $\mathscr{H}_\mathscr{S} \otimes \mathbb{C}[\psi_{\mathscr{E}_1} \otimes \psi_{\mathscr{E}_2} \otimes \cdots]$, and define, analogously to (18)

$$M_m = P \mathrm{e}^{\mathrm{i}K_m} P,$$

which we identify with an operator on $\mathrm{Ran}\, P = \mathscr{H}_\mathscr{S}$. Suppose that we start initially in the state $\psi_0 = \psi_\mathscr{S} \otimes \psi_\mathscr{E}$, where $\psi_\mathscr{E} = \psi_{\mathscr{E}_1} \otimes \psi_{\mathscr{E}_2} \otimes \cdots$. One shows that the

expectation value of an observable $A \in \mathfrak{M}_{\mathscr{S}}$ at step m is given by

$$\left\langle \psi_0, \alpha_{\mathrm{RI}}^m(A)\psi_0 \right\rangle = \langle \psi_0, M_1 \cdots M_m A \psi_0 \rangle \,,$$

see the proof of Theorem 3 in Sect. 5, and [4, 5]. We thus see that in order to study the asymptotics of the dynamics, we must consider products $M_1 \cdots M_m$. Two crucial properties of the operators M_k are

1. $M_1 \cdots M_m$ is bounded, uniformly in the number of factors m.
2. The M_k have a common invariant vector, $M_k \psi_{\mathscr{S}} = \psi_{\mathscr{S}}$, for all k.

The former fact follows quite easily from the fact that the M_k implement a dynamics which is norm-preserving, see e.g. [4, 5]. The latter fact follows directly from the construction of the operators M_k. In the random setting, we shall consider the M_k to be a family of independent, identically distributed random matrices, called $M(\omega)$.

3.2 Results

We introduce a general class of random matrices having the two properties mentioned above. Let $M(\omega)$ be a random matrix on $\mathbb{C}^d$, with probability space $(\Omega, \mathscr{F}, \mathrm{p})$. We say that $M(\omega)$ is a *random reduced dynamics operator* (RRDO) if

(1) There exists a norm $|||\cdot|||$ on $\mathbb{C}^d$ such that, for all ω, $M(\omega)$ is a contraction on $\mathbb{C}^d$ endowed with the norm $|||\cdot|||$.
(2) There is a vector $\psi_{\mathscr{S}}$, constant in ω, such that $M(\omega)\psi_{\mathscr{S}} = \psi_{\mathscr{S}}$, for all ω.

Note that (1) is equivalent to the property 1 from in the previous section. We normalize $\psi_{\mathscr{S}}$ as $\|\psi_{\mathscr{S}}\| = 1$, where $\|\cdot\|$ denotes the Euclidean norm. To an RRDO $M(\omega)$, we associate the (iid) *random reduced dynamics process* (RRDP)

$$\Psi_n(\overline{\omega}) := M(\omega_1) \cdots M(\omega_n), \qquad \overline{\omega} \in \Omega^{\mathbb{N}^*}.$$

We will show that Ψ_n has a decomposition into an exponentially decaying part and a fluctuating part. To identify these parts, we proceed as follows. It follows from (1) and (2) that the spectrum of an RRDO $M(\omega)$ must lie inside the closed complex unit disk, and that 1 is an eigenvalue (with eigenvector $\psi_{\mathscr{S}}$). Let $P_1(\omega)$ denote the spectral projection of $M(\omega)$ corresponding to the eigenvalue 1 ($\dim P_1(\omega) \geq 1$), and let $P_1^*(\omega)$ be its adjoint operator. Define

$$\psi(\omega) := P_1(\omega)^* \psi_{\mathscr{S}}, \tag{35}$$

and set

$$P(\omega) = |\psi_{\mathscr{S}}\rangle\langle\psi(\omega)|.$$

For $\psi, \phi \in \mathbb{C}^d$, we denote by $|\psi\rangle\langle\phi|$ the rank-one operator $|\psi\rangle\langle\phi|\chi = \langle\phi, \chi\rangle\,\psi$, and our convention is to take the inner products linear in the second factor. We put

$$Q(\omega) = \mathbb{1} - P(\omega).$$

Note that the vector $\psi(\omega)$ is normalized as $\langle \psi_{\mathscr{S}}, \psi(\omega)\rangle = 1$. We decompose $M(\omega)$ as

$$M(\omega) = P(\omega) + Q(\omega)M(\omega)Q(\omega) =: P(\omega) + M_Q(\omega). \tag{36}$$

Taking into account this decomposition, one easily shows the following result.

Proposition 5 ([5]). *We have*

$$\Psi_n(\overline{\omega}) := M(\omega_1)\cdots M(\omega_n) = |\psi_{\mathscr{S}}\rangle\langle\theta_n(\overline{\omega})| + M_Q(\omega_1)\cdots M_Q(\omega_n), \tag{37}$$

where $\theta_n(\overline{\omega})$ is the Markov process

$$\theta_n(\overline{\omega}) = M^*(\omega_n)\cdots M^*(\omega_2)\psi(\omega_1), \tag{38}$$

$M^*(\omega_j)$ being the adjoint operator of $M(\omega_j)$.

We analyze the two parts in the r.h.s. of (37) separately. Let $\mathscr{M}_{(E)}$ be the set of RRDOs M whose spectrum on the complex unit circle consists only of a simple eigenvalue $\{1\}$. On $\Omega^{\mathbb{N}^*}$ we define the probability measure $\mathrm{d}\mathbb{P}$ in a standard fashion by

$$\mathrm{d}\mathbb{P} = \Pi_{j\geq 1}\mathrm{d}p_j, \quad \text{where} \quad \mathrm{d}p_j \equiv \mathrm{d}p, \ \forall j \in \mathbb{N}^*.$$

Theorem 6 (Decaying process, [5]). *Let $M(\omega)$ be a random reduced dynamics operator. Suppose that $\mathrm{p}(M(\omega) \in \mathscr{M}_{(E)}) > 0$. Then there exist a set $\Omega_1 \subset \Omega^{\mathbb{N}^*}$ and constants $C, \alpha > 0$, s.t. $\mathbb{P}(\Omega_1) = 1$ and s.t. for any $\overline{\omega} \in \Omega_1$ and any $n \geq 1$,*

$$\|M_Q(\omega_1)\cdots M_Q(\omega_n)\| \leq C\mathrm{e}^{-\alpha n}. \tag{39}$$

Remarks. 1. In the case where $M(\omega) = M$ is constant, and $M \in \mathscr{M}_{(E)}$, one readily shows that for any $\epsilon > 0$ there is a C_ϵ such that $\|(M_Q)^n\| \leq C_\epsilon \mathrm{e}^{-n(\gamma-\epsilon)}$, for all $n \geq 0$, and where $\gamma = \min_{z\in\mathrm{spec}(M)\setminus\{1\}} |\log|z||$ (see e.g. also Proposition 2). It is remarkable that in the random case, the mere condition of M having an arbitrarily small, non-vanishing probability to be in $\mathscr{M}_{(E)}$ suffices to guarantee the exponential decay of the product in (39).

2. Any stochastic matrix whose entries are all nonzero belongs to $\mathscr{M}_{(E)}$.

3. If $\{1\}$ is a simple eigenvalue of $M(\omega)$ then the decomposition (36) is just the spectral decomposition of the matrix $M(\omega)$.

4. The choice (35) ensures that $\psi(\omega)$ is an eigenvector of $M^*(\omega)$. Other choices of measurable $\psi(\omega)$ which are bounded in ω lead to different decompositions of $M(\omega)$, and can be useful as well. For instance, if $M(\omega)$ is a bistochastic matrix, then one can take for $\psi(\omega)$ an $M^*(\omega)$-invariant vector which is constant in ω.

Our next result concerns the asymptotics of the Markov process (38). Set $\mathbb{E}[f] = \int_\Omega f(\omega)\mathrm{d}p(\omega)$ for a random variable f, and denote by $P_{1,\mathbb{E}[M]}$ the spectral projection of $\mathbb{E}[M]$ onto the eigenvalue $\{1\}$.

Theorem 7 (Fluctuating process, [5]). *Let $M(\omega)$ be a random reduced dynamics operator. Suppose that $\mathrm{p}(M(\omega) \in \mathscr{M}_{(E)}) > 0$. Then we have $\mathbb{E}[M] \in \mathscr{M}_{(E)}$. Moreover, there exists a set $\Omega_2 \subset \Omega^{\mathbb{N}^*}$ s.t. $\mathbb{P}(\Omega_2) = 1$ and, for all $\overline{\omega} \in \Omega_2$,*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} \theta_n(\overline{\omega}) = \theta, \tag{40}$$

where

$$\theta = \left(\mathbb{1} - \mathbb{E}[M_Q]^*\right)^{-1} \mathbb{E}[\psi] = P^*_{1,\mathbb{E}[M]}\mathbb{E}[\psi] = P^*_{1,\mathbb{E}[M]}\psi_{\mathscr{S}}. \tag{41}$$

Remarks. 5. In the case where M is constant in ω, we have $\mathbb{E}[M_Q]^* = (M_Q)^*$, $\mathbb{E}[\psi] = \psi$, and under the assumption of Theorem 7, that $M \in \mathscr{M}_{(E)}$. Therefore, $P_1 = P = |\psi_{\mathscr{S}}\rangle\langle\psi|$ and hence $Q^*\psi = 0$, and $(M_Q)^*\psi = 0$. Consequently, we have $\theta = \psi$. This coincides with the results of Theorem 3. However, the latter equality is not satisfied for general, ω-dependent matrices M, as is shown in [5].

6. The ergodic average limit of $\theta_n(\overline{\omega})$ does not depend on the particular choice of $\psi(\omega)$. This follows from the last equality in (41).

7. We show in [5] that for every *fixed* $\overline{\omega}$, $\theta_n(\overline{\omega})$ converges if and only if $\psi(\omega_n)$ converges, and that the limits coincide if they exist.

Combining Theorems 6 and 7 we obtain the following result.

Theorem 8 (Ergodic theorem for RRDP, [5]). *Let $M(\omega)$ be a random reduced dynamics operator. Suppose $\mathrm{p}(M(\omega) \in \mathscr{M}_{(E)}) > 0$. Then there exists a set $\Omega_3 \subset \Omega^{\mathbb{N}^*}$ s.t. $\mathbb{P}(\Omega_3) = 1$ and, for all $\overline{\omega} \in \Omega_3$,*

$$\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} M(\omega_1)\cdots M(\omega_n) = |\psi_{\mathscr{S}}\rangle\langle\theta| = P_{1,\mathbb{E}[M]}. \tag{42}$$

Remark. 8. If one can choose $\psi(\omega) \equiv \psi$ to be independent of ω (see also Remark 4 above), then one can show (see [5]) that $\theta_n(\overline{\omega}) = \psi$, for all $n, \overline{\omega}$. It thus follows from (37)–(39) that $\lim_{n\to\infty} M(\omega_1)\cdots M(\omega_n) = |\psi_{\mathscr{S}}\rangle\langle\psi|$, a.s., exponentially fast.

4 An Example: Spins

We consider a model in which the small system as well as the elements of the chain are 2-level systems. Such models (or more generally, a d-level system interacting with a chain of n-level systems, a situation we could equally well treat here) have been considered previously in [1].

Consider the trace state on a two-level system, $\varrho_\infty(A) = \frac{1}{2}\mathrm{Tr}(A)$, where $A \in M_2(\mathbb{C})$ is a 2×2 matrix, and the trace is taken over $\mathbb{C}^2$. In order to represent ϱ_∞ by a vector state, we must perform the *Gelfand-Naimark-Segal* construction. The representation Hilbert space is $\mathbb{C}^2 \otimes \mathbb{C}^2$, and we have

$$\varrho_\infty(A) = \langle \psi_\infty, (A \otimes \mathbb{1})\psi_\infty \rangle,$$

where the inner product is that of $\mathbb{C}^2 \otimes \mathbb{C}^2$ and where $\psi_\infty = \frac{1}{\sqrt{2}}[\varphi_1 \otimes \varphi_1 + \varphi_2 \otimes \varphi_2]$, with

$$\varphi_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \text{and} \quad \varphi_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

This representation serves to represent the mixed state ϱ_∞ by a vector state in an "enlarged" Hilbert space. The von Neumann algebra of observables for the small system and for the elements of the chain are

$$\mathfrak{M}_{\mathscr{S}} = \mathfrak{M}_{\mathscr{E}} = M_2(\mathbb{C}) \otimes \mathbb{1} = \{A \otimes \mathbb{1} | A \in M_2(\mathbb{C})\}, \tag{43}$$

acting on the Hilbert space $\mathscr{H}_{\mathscr{S}} = \mathscr{H}_{\mathscr{E}} = \mathbb{C}^2 \otimes \mathbb{C}^2$. Let $E_{\mathscr{S}}, E_{\mathscr{E}} > 0$ be the "excited" energy levels of the small system and the elements of the chain, respectively. The dynamics are given by

$$\alpha^t_{\mathscr{S}}(A \otimes \mathbb{1}) = \mathrm{e}^{\mathrm{i}th_{\mathscr{S}}} A \mathrm{e}^{-\mathrm{i}th_{\mathscr{S}}} \otimes \mathbb{1}, \quad \text{and} \quad \alpha^t_{\mathscr{E}}(A \otimes \mathbb{1}) = \mathrm{e}^{\mathrm{i}th_{\mathscr{E}}} A \mathrm{e}^{-\mathrm{i}th_{\mathscr{E}}} \otimes \mathbb{1}, \tag{44}$$

where

$$h_{\mathscr{S}} = \begin{bmatrix} 0 & 0 \\ 0 & E_{\mathscr{S}} \end{bmatrix}, \qquad h_{\mathscr{E}} = \begin{bmatrix} 0 & 0 \\ 0 & E_{\mathscr{E}} \end{bmatrix}.$$

We choose the reference state $\psi_{\mathscr{S}}$ to be the tracial state ψ_∞ defined above. The associated Liouville operator is $L_{\mathscr{S}} = h_{\mathscr{S}} \otimes \mathbb{1} - \mathbb{1} \otimes h_{\mathscr{S}}$, and the modular conjugation and modular operator associated to $(\mathfrak{M}_{\mathscr{S}}, \psi_{\mathscr{S}})$ are

$$J_{\mathscr{S}}(\phi \otimes \chi) = \chi \otimes \bar{\phi}, \quad \Delta_{\mathscr{S}} = \mathbb{1} \otimes \mathbb{1}, \tag{45}$$

where $\bar{\phi}$ denotes entrywise complex conjugation (in the canonical basis).

In order to avoid confusion between the small system and elements of the chain, we denote by $\phi_{ij} = \phi_i \otimes \phi_j$ the basis of $\mathscr{H}_{\mathscr{E}}$. We take the reference state of $\mathscr{E}$ to be the $(\alpha^t_{\mathscr{E}}, \beta)$-KMS state. Its representative vector is

$$\psi_{\mathscr{E}} = \frac{1}{\sqrt{1 + \mathrm{e}^{-\beta E_{\mathscr{E}}}}} (\phi_{11} + \mathrm{e}^{-\beta E_{\mathscr{E}}/2} \phi_{22}). \tag{46}$$

The standard Liouville operator is $L_{\mathscr{E}} = h_{\mathscr{E}} \otimes \mathbb{1} - \mathbb{1} \otimes h_{\mathscr{E}}$, and the modular conjugation and modular operator associated to $(\mathfrak{M}_{\mathscr{E}}, \psi_{\mathscr{E}})$ are

$$J_{\mathscr{E}}(\phi \otimes \chi) = \chi \otimes \bar{\phi}, \quad \Delta_{\mathscr{E}} = \mathrm{e}^{-\beta L_{\mathscr{E}}}. \tag{47}$$

We now describe the interaction between $\mathscr{S}$ and $\mathscr{E}$. Let us denote by a and a^* the annihilation and creation operators,

$$a_\# = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad a^*_\# = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix},$$

where $\# = \mathscr{S}, \mathscr{E}$. Let $a, b, c, d \in \mathbb{C}$ and set

$$I = \begin{bmatrix} a & b \\ c & d \end{bmatrix}.$$

The interaction operator, acting on $\mathscr{H}_{\mathscr{S}} \otimes \mathscr{H}_{\mathscr{E}} = \mathbb{C} \otimes \mathbb{C} \otimes \mathbb{C} \otimes \mathbb{C}$ is then defined as

$$V = I \otimes \mathbb{1} \otimes a^* \otimes \mathbb{1} + I^* \otimes \mathbb{1} \otimes a \otimes \mathbb{1}. \tag{48}$$

The standard Liouville operator, generating the interacting dynamics, is the self-adjoint operator

$$L_\lambda := L_{\mathscr{S}} + L_{\mathscr{E}} + \lambda V, \tag{49}$$

where λ is a real coupling constant. In this setting, we have

$$M_{\lambda=0} = P \mathrm{e}^{\mathrm{i}\tau L_{\mathscr{S}}} P,$$

and we will always assume that $\tau E_{\mathscr{S}} \notin \pi\mathbb{Z}$, in order to ensure that the spectrum of $M_{\lambda=0}$ is nondegenerate. This assumption is made for convenience, and can most probably be lifted.

The operator K associated to L_λ and the reference state $\psi_{\mathscr{S}} \otimes \psi_{\mathscr{E}} \otimes \psi_{\mathscr{E}} \cdots$ (see (15)) is

$$K_\lambda := L_{\mathscr{S}} + L_{\mathscr{E}} + \lambda(V - J\Delta^{1/2} V \Delta^{-1/2} J) = K_0 + \lambda W. \tag{50}$$

We consider the following assumptions on the effectiveness of the coupling operator, where τ denotes the interaction time.

(S1) $b \neq 0$ and $\tau(E_{\mathscr{E}} - E_{\mathscr{S}}) \notin 2\pi\mathbb{Z}$.
(S2) $c \neq 0$ and $\tau(E_{\mathscr{E}} + E_{\mathscr{S}}) \notin 2\pi\mathbb{Z}$.

The proof of the following result is based on perturbation theory in λ. We outline it in Sect. 5. Set $\mathrm{sinc}(x) = \sin(x)/x$.

Theorem 9 (Deterministic spin model [4]). *Suppose that $\tau E_{\mathscr{E}} \notin \pi\mathbb{Z}$ and that either Assumption* (S1) *or* (S2) *is satisfied. Then, there exists $\lambda_0 > 0$ such that for all $0 < |\lambda| < \lambda_0$, the operator $M_\lambda := P\mathrm{e}^{\mathrm{i}\tau K_\lambda} P$ satisfies the ergodic assumption* (E). *In particular the spin-spin system satisfies Theorem 3, with $\gamma \geq \gamma_0 \lambda^2 + O(\lambda^4)$. Moreover, the asymptotic state $\varrho_{+,\lambda}$ is given by*

$$\varrho_{+,\lambda}(A_{\mathscr{S}}) = \frac{1}{\alpha_1 + \alpha_2} \langle \alpha_1 \psi_{11} + \alpha_2 \psi_{22}, A_{\mathscr{S}}(\psi_{11} + \psi_{22}) \rangle + O(\lambda^2), \tag{51}$$

where

$$\alpha_1 := |b|^2 \mathrm{sinc}^2\left[\frac{\tau(E_{\mathscr{E}} - E_{\mathscr{S}})}{2}\right] + \mathrm{e}^{-\beta E_{\mathscr{E}}} |c|^2 \mathrm{sinc}^2\left[\frac{\tau(E_{\mathscr{E}} + E_{\mathscr{S}})}{2}\right],$$

$$\alpha_2 := \mathrm{e}^{-\beta E_{\mathscr{E}}} |b|^2 \mathrm{sinc}^2\left[\frac{\tau(E_{\mathscr{E}} - E_{\mathscr{S}})}{2}\right] + |c|^2 \mathrm{sinc}^2\left[\frac{\tau(E_{\mathscr{E}} + E_{\mathscr{S}})}{2}\right],$$

$$\gamma_0 := \tau^2 \min\left[\frac{\alpha_1 + \alpha_2}{1 + \mathrm{e}^{-\beta E_{\mathscr{E}}}}, \frac{1}{2}\frac{\alpha_1 + \alpha_2}{1 + \mathrm{e}^{-\beta E_{\mathscr{E}}}} + \frac{|a-d|^2}{2} \mathrm{sinc}^2\left(\frac{\tau E_{\mathscr{E}}}{2}\right)\right].$$

Assumptions (S1), (S2) serve to ensure that $\gamma_0 > 0$. Indeed, if (S1) is satisfied, then $\alpha_1 > 0$, if (S2) is satisfied, then $\alpha_2 > 0$.

Recall that we denote by $\mathscr{M}_{(E)}$ the set of matrices M whose spectrum on the complex unit circle consists only of a simple eigenvalue 1 (cf. after (38)). The next result gives an explicit bound on the coupling constant λ which ensures that M is in $\mathscr{M}_{(E)}$. We give a proof in Sect. 5.

Lemma 10. *Suppose that*

$$\lambda_0^2 := \frac{1}{2\cosh(\|W\|\tau)}\left[|b|^2\,\frac{\sin^2(\tau(E_{\mathscr{E}}-E_{\mathscr{S}})/2)}{(E_{\mathscr{E}}-E_{\mathscr{S}})^2}+|c|^2\,\frac{\sin^2(\tau(E_{\mathscr{E}}+E_{\mathscr{S}})/2)}{(E_{\mathscr{E}}+E_{\mathscr{S}})^2}\right] > 0.$$

If $0 < |\lambda| < \lambda_0$, *then* $M_\lambda \in \mathscr{M}_{(E)}$.

Let us now consider the same system, but with a random interaction time $\tau = \tau(\omega)$. (The following analysis extends pretty effortlessly to more general settings, where e.g. also the temperature β, the energies $E_{\mathscr{E}}$, $E_{\mathscr{S}}$, or the coefficients a, b, c, d, of the interaction matrix are random, cf. [6].) Consider the conditions

(S3) $b \neq 0$ and there is an $\eta_- > 0$, s.t.

$$\mathrm{p}\big(\tau E_{\mathscr{E}} \notin \pi\mathbb{Z},\ |\tau[E_{\mathscr{E}}-E_{\mathscr{S}}]/2-\pi\mathbb{Z}| \geq \eta_-\big) > 0.$$

(S4) $c \neq 0$ and there is an $\eta_+ > 0$, s.t.

$$\mathrm{p}\big(\tau E_{\mathscr{E}} \notin \pi\mathbb{Z},\ |\tau[E_{\mathscr{E}}+E_{\mathscr{S}}]/2-\pi\mathbb{Z}| \geq \eta_+\big) > 0.$$

Again, the condition $\tau E_{\mathscr{E}} \notin \pi\mathbb{Z}$ is imposed so that $M_{\lambda=0}$ has simple spectrum, which makes the calculations in the perturbation theory somewhat simpler. This condition can most probably be dropped.

Theorem 11 (Random spin model). *Suppose that either*

1. *Condition* (S3) *is satisfied, and*

$$0 < \lambda^2 < \frac{|b|^2}{2\cosh(2\eta_-\|W\|\,|E_{\mathscr{E}}-E_{\mathscr{S}}|^{-1})}\,\frac{\sin^2(\eta_-)}{(E_{\mathscr{E}}-E_{\mathscr{S}})^2},$$

or

2. *Condition* (S4) *is satisfied, and*

$$0 < \lambda^2 < \frac{|c|^2}{2\cosh(2\eta_+\|W\|\,|E_{\mathscr{E}}+E_{\mathscr{S}}|^{-1})}\,\frac{\sin^2(\eta_+)}{(E_{\mathscr{E}}+E_{\mathscr{S}})^2}.$$

Then the results of Theorems 6–8 hold.

We prove this result in Sect. 5.

5 Some Proofs

Outline of the Proof of Theorem 3

We outline the proof for the special case where $\varrho_+(\cdot) = \langle \psi_0, \cdot\, \psi_0\rangle$, where $\psi_0 = \psi_{\mathscr{S}} \otimes_{k\geq 1} \psi_{\mathscr{E}}$, and for observables $A_{\mathscr{S}} \in \mathfrak{M}_{\mathscr{S}}$. Recall that

$$\alpha^t_{\rm RI}(A_{\mathscr{S}}) = \mathrm{e}^{\mathrm{i}\tau \widetilde{L}_1} \cdots \mathrm{e}^{\mathrm{i}\tau \widetilde{L}_m} \mathrm{e}^{\mathrm{i}s\widetilde{L}_{m+1}} A_{\mathscr{S}} \mathrm{e}^{-\mathrm{i}s\widetilde{L}_{m+1}} \mathrm{e}^{-\mathrm{i}\tau \widetilde{L}_m} \cdots \mathrm{e}^{-\mathrm{i}\tau \widetilde{L}_1}. \tag{52}$$

The proof of Theorem 3 has four main ingredients.

1. *Factorization of the free dynamics*. Taking into account the decomposition (11) of $\widetilde{L}_k$, we see that

$$\mathrm{e}^{-\mathrm{i}s\widetilde{L}_{m+1}} \mathrm{e}^{-\mathrm{i}\tau \widetilde{L}_m} \cdots \mathrm{e}^{-\mathrm{i}\tau \widetilde{L}_1} = U_m^- \mathrm{e}^{-\mathrm{i}sL_{m+1}} \mathrm{e}^{-\mathrm{i}\tau L_m} \cdots \mathrm{e}^{-\mathrm{i}\tau L_1} U_m^+,$$

   where $U_m^\pm$ are the unitaries

$$U_m^- = \exp\Big[-\mathrm{i}\sum_{j=1}^{m}[(m-j)\tau + s]L_{\mathscr{E},j}\Big],$$

$$U_m^+ = \exp\Big[-\mathrm{i}\sum_{j=2}^{m+1}(j-1)\tau L_{\mathscr{E},j} - \mathrm{i}(m\tau + s)\sum_{j\geq m+1} L_{\mathscr{E},j}\Big].$$

   Clearly, $U_m^\pm \psi_0 = \psi_0$, for all m, so (52) gives

$$\big\langle \psi_0, \alpha^t_{\rm RI}(A_{\mathscr{S}})\psi_0\big\rangle = \big\langle \psi_0, \mathrm{e}^{\mathrm{i}\tau L_1} \cdots \mathrm{e}^{\mathrm{i}sL_{m+1}} A_{\mathscr{S}} \mathrm{e}^{-\mathrm{i}sL_{m+1}} \cdots \mathrm{e}^{-\mathrm{i}\tau L_1}\psi_0\big\rangle. \tag{53}$$

2. *Passage to non-self-adjoint generator of dynamics*. We now employ a trick that has been recently invented to analyze the asymptotics of open quantum systems far from equilibrium [7, 9]. We replace the operators L_m by operators K_m, having the property that K_m implements the same dynamics as L_m, but satisfies in addition the property $K_m\psi_0 = 0$. The existence of such operators is linked to the deep Tomita-Takesaki theory of von Neumann algebras, and in fact, K_m is expressed in terms of the modular data (J, Δ) associated to the pair $(\mathfrak{M}, \psi_0)$, [3]. It is given explicitly by (36). We thus obtain from (53)

$$\big\langle \psi_0, \alpha^t_{\rm RI}(A_{\mathscr{S}})\psi_0\big\rangle = \big\langle \psi_0, \mathrm{e}^{\mathrm{i}\tau K_1} \cdots \mathrm{e}^{\mathrm{i}\tau K_m} \mathrm{e}^{\mathrm{i}sK_{m+1}} A_{\mathscr{S}}\psi_0\big\rangle. \tag{54}$$

3. *Reduction of the dynamics*. In this step we take advantage of the fact that the elements $\mathscr{E}$ in the chain $\mathscr{C}$ are independently prepared (not entangled) and dynamically not directly coupled. Let P be the orthogonal projection onto $\mathscr{H}_{\mathscr{S}} \otimes \psi_{\mathscr{C}}$, where $\psi_{\mathscr{C}} = \psi_{\mathscr{E}} \otimes \psi_{\mathscr{E}} \otimes \cdots$. Then $A_{\mathscr{S}}\psi_0 = A_{\mathscr{S}}P\psi_0 = PA_{\mathscr{S}}\psi_0$ (since $\psi_0 = P\psi_0$, and $A_{\mathscr{S}} \in \mathfrak{M}_{\mathscr{S}}$), so we are led to consider $P\mathrm{e}^{\mathrm{i}\tau K_1} \cdots \mathrm{e}^{\mathrm{i}\tau K_m} \mathrm{e}^{\mathrm{i}sK_{m+1}} P$. Writing $P = P_{\psi_{\mathscr{E}}} \otimes P_{\psi_{\mathscr{E}}} \otimes \cdots$, where $\psi_{\mathscr{E}} = |\psi_{\mathscr{E}}\rangle\langle\psi_{\mathscr{E}}|$, we note that

$$e^{isK_{m+1}}P = (P_{\psi_{\mathscr{E}}} \otimes \cdots P_{\psi_{\mathscr{E}}} \otimes P_{\psi_{\mathscr{E}}} \otimes \mathbb{1} \otimes P_{\psi_{\mathscr{E}}} \otimes \cdots)e^{isK_{m+1}}P, \tag{55}$$

where the identity operator stands at the spot $(m+1)$. This follows simply because K_{m+1} acts non-trivially only on the factor $(m+1)$ on the chain. On the other hand, for the same reason, we have

$$Pe^{i\tau K_1}\cdots e^{i\tau K_m} = Pe^{i\tau K_1}\cdots e^{i\tau K_m}(\mathbb{1}\otimes\mathbb{1}\cdots\otimes\mathbb{1}\otimes P_{\psi_{\mathscr{E}}}\otimes P_{\psi_{\mathscr{E}}}\otimes\cdots), \tag{56}$$

where the first nontrivial projection on the right is on factor $m+1$. The combination of (55) and (56) gives

$$Pe^{i\tau K_1}\cdots e^{i\tau K_m}e^{isK_{m+1}}P = Pe^{i\tau K_1}P\cdots Pe^{i\tau K_m}Pe^{isK_{m+1}}P. \tag{57}$$

Since the interaction is the same at each step in the repeated interaction process, we can identify the operator

$$Pe^{i\tau L_k}P \equiv M$$

as an operator on $\mathscr{H}_{\mathscr{S}}$, independent of k. Thus, with (54) and (57), we obtain

$$\langle\psi_0, \alpha^t_{\mathrm{RI}}(A_{\mathscr{S}})\psi_0\rangle = \langle\psi_0, M^{m(t)}Pe^{is(t)K}PA_{\mathscr{S}}\psi_0\rangle, \tag{58}$$

where we also set $Pe^{is(t)K_k}P = Pe^{is(t)K}P$, for any k. The dynamical process is now clear: the term $M^{m(t)}$ will have a limit as $t\to\infty$ (under suitable conditions), while $Pe^{is(t)K}P$ is oscillating in t (with period τ).

4. *Spectral analysis of M and decay of $M^{m(t)}$.* Proposition 2 shows that

$$\left|\langle\psi_0, \alpha^t_{\mathrm{RI}}(A_{\mathscr{S}})\psi_0\rangle - \langle\psi^*_{\mathscr{S}}, \alpha^{s(t)}_{\mathrm{RI}}(A_{\mathscr{S}})\psi_{\mathscr{S}}\rangle\right| \le C_\epsilon e^{-t(\gamma-\epsilon)/\tau},$$

where we have taken into account that

$$\langle\psi_0, Pe^{is(t)K}PA_{\mathscr{S}}\psi_0\rangle = \langle\psi_0, Pe^{is(t)L}A_{\mathscr{S}}e^{-is(t)L}\psi_0\rangle = \langle\psi_0, \alpha^{s(t)}_{\mathrm{RI}}(A_{\mathscr{S}})\psi_0\rangle.$$

This concludes the proof of Theorem 6 in the special setting.

Outline of the Proof of Theorem 9

A Dyson expansion gives

$$\begin{aligned} e^{i\tau K_\lambda} = {} & e^{i\tau K_0} + i\lambda\int_0^\tau dt e^{i(\tau-t)K_0}We^{itK_0} \\ & - \lambda^2\int_0^\tau\int_0^t e^{i(\tau-t)K_0}We^{i(t-s)K_0}We^{isK_0}\,ds\,dt + R(\tau,\lambda), \end{aligned} \tag{59}$$

where

$$R(\tau,\lambda) = \sum_{n\geq 2}(-\lambda)^{2n}\int_0^\tau \mathrm{d}t_1\cdots\int_0^{t_{2n-1}}\mathrm{d}t_{2n}\; P\mathrm{e}^{\mathrm{i}t_1K_0}W\mathrm{e}^{-\mathrm{i}t_1K_0}\cdots\mathrm{e}^{\mathrm{i}t_{2n}K_0}W\mathrm{e}^{-\mathrm{i}t_{2n}K_0}P. \tag{60}$$

After a somewhat lengthy but straightforward computation, one obtains a perturbative expression for the operator $M(\lambda) = P\mathrm{e}^{\mathrm{i}\tau K_\lambda}P$, and the following expansions for the three eigenvalues $e_0(\lambda)$, $e_\pm(\lambda)$ of $M(\lambda)$, other than the eigenvalue 1:

$$\begin{aligned}
e_0(\lambda) &= 1 - \frac{\lambda^2\tau^2}{1+\mathrm{e}^{-\beta E_{\mathscr{E}}}}(\alpha_1+\alpha_2) + O(\lambda^4)\\
e_+(\lambda) &= \mathrm{e}^{\mathrm{i}\tau E_{\mathscr{S}}}\Bigg[1 - \frac{\lambda^2\tau^2}{2(1+\mathrm{e}^{-\beta E_{\mathscr{E}}})}\Bigg(\alpha_1+\alpha_2+(1+\mathrm{e}^{-\beta E_{\mathscr{E}}})|a-d|^2\\
&\quad\times\mathrm{sinc}^2\Big(\frac{\tau E_{\mathscr{E}}}{2}\Big)\Bigg)\\
&\quad+\mathrm{i}\frac{\lambda^2\tau^2}{1+\mathrm{e}^{-\beta E_{\mathscr{E}}}}\Bigg((1-\mathrm{e}^{-\beta E_{\mathscr{E}}})(|a|^2-|d|^2)\frac{1-\mathrm{sinc}(\tau E_{\mathscr{E}})}{\tau E_{\mathscr{E}}}\\
&\quad+(1-\mathrm{e}^{-\beta E_{\mathscr{E}}})\,\mathrm{Im}(\bar{a}d)\mathrm{sinc}^2\Big(\frac{\tau E_{\mathscr{E}}}{2}\Big)\\
&\quad-(1+\mathrm{e}^{-\beta E_{\mathscr{E}}})|b|^2\frac{1-\mathrm{sinc}(\tau(E_{\mathscr{E}}-E_{\mathscr{S}}))}{\tau(E_{\mathscr{E}}-E_{\mathscr{S}})}\\
&\quad+(1+\mathrm{e}^{-\beta E_{\mathscr{E}}})|c|^2\frac{1-\mathrm{sinc}(\tau(E_{\mathscr{E}}+E_{\mathscr{S}}))}{\tau(E_{\mathscr{E}}+E_{\mathscr{S}})}\Bigg)\Bigg] + O(\lambda^4)\\
e_-(\lambda) &= \mathrm{e}^{-\mathrm{i}\tau E_{\mathscr{S}}}\Bigg[1 - \frac{\lambda^2\tau^2}{2(1+\mathrm{e}^{-\beta E_{\mathscr{E}}})}\Bigg(\alpha_1+\alpha_2+(1+\mathrm{e}^{-\beta E_{\mathscr{E}}})|a-d|^2\\
&\quad\times\mathrm{sinc}^2\Big(\frac{\tau E_{\mathscr{E}}}{2}\Big)\Bigg)\\
&\quad+\mathrm{i}\frac{\lambda^2\tau^2}{1+\mathrm{e}^{-\beta E_{\mathscr{E}}}}\Bigg((1-\mathrm{e}^{-\beta E_{\mathscr{E}}})(|d|^2-|a|^2)\frac{1-\mathrm{sinc}(\tau E_{\mathscr{E}})}{\tau E_{\mathscr{E}}}\\
&\quad+(1-\mathrm{e}^{-\beta E_{\mathscr{E}}})\,\mathrm{Im}(a\bar{d})\,\mathrm{sinc}^2\Big(\frac{\tau E_{\mathscr{E}}}{2}\Big)\\
&\quad+(1+\mathrm{e}^{-\beta E_{\mathscr{E}}})|b|^2\frac{1-\mathrm{sinc}(\tau(E_{\mathscr{E}}-E_{\mathscr{S}}))}{\tau(E_{\mathscr{E}}-E_{\mathscr{S}})}\\
&\quad-(1+\mathrm{e}^{-\beta E_{\mathscr{E}}})|c|^2\frac{1-\mathrm{sinc}(\tau(E_{\mathscr{E}}+E_{\mathscr{S}}))}{\tau(E_{\mathscr{E}}+E_{\mathscr{S}})}\Bigg)\Bigg] + O(\lambda^4).
\end{aligned} \tag{61}$$

These expressions show that we have

$$|\log|e_0(\lambda)|| \geq \frac{\lambda^2\tau^2}{1+\mathrm{e}^{-\beta E_{\mathscr{E}}}}(\alpha_1+\alpha_2) + O(\lambda^4),$$

$$|\log|e_{\pm}(\lambda)|| \geq \frac{\lambda^2\tau^2}{2(1+\mathrm{e}^{-\beta E_{\mathscr{E}}})}\left(\alpha_1+\alpha_2+(1+\mathrm{e}^{-\beta E_{\mathscr{E}}})|a-d|^2\mathrm{sinc}^2\left(\frac{\tau E_{\mathscr{E}}}{2}\right)\right) + O(\lambda^4).$$

Therefore, $\min_{z\in\mathrm{spec}(M)\setminus\{1\}}|\log|z||\geq\lambda^2\gamma_0+O(\lambda^4)$, where γ_0 is as in Theorem 9.

In order to calculate the asymptotic state $\varrho_{+,\lambda}$, (51), one performs perturbation theory in the formula (22). We do not present the calculations here.

Proof of Lemma 10. We need to show that $|e_0(\lambda)|$, $|e_{\pm}(\lambda)|<1$, where $e_0(\lambda)$, $e_{\pm}(\lambda)$ are given in (61). The error term in those expressions are bounded above by $\|R(\tau,\lambda)\|$, cf. (59) and (60) (and [8], II.3, Theorem 3.9). We have ($|\lambda|\leq 1$)

$$\|R(\tau,\lambda)\|\leq\sum_{n\geq 2}\lambda^{2n}\|W\|^{2n}\frac{\tau^{2n}}{(2n!)}\leq\lambda^4\cosh(\|W\|\tau).$$

To ensure that $|e_0(\lambda)|<1$, we thus impose the condition

$$\lambda^2\cosh(\|W\|\tau)<\frac{1}{2}\frac{\tau^2(\alpha_1+\alpha_2)}{1+\mathrm{e}^{-\beta E_{\mathscr{E}}}},$$

which is equivalent to $|\lambda|<\lambda_0$. Next, we want to impose $|e_{\pm}(\lambda)|<1$. We write $|e_{\pm}|=|1-x+\mathrm{i}y+\xi|$, where $x\geq 0$, $y\in\mathbb{R}$ and $\xi\in\mathbb{C}$ are read off the expression for $e_{\pm}$ given in (61). Here, $-x+\mathrm{i}y$ are the terms of order λ^2 coming from the Dyson series expansion, and ξ incorporates all higher order terms (orders ≥ 4). It is sufficient to impose the condition $|\xi|<1-|1-x+\mathrm{i}y|$ in order to ensure that $|e_{\pm}|<1$. Using that $x^2+y^2\leq[\lambda^2\|W\|^2\tau^2/2]^2$, one easily sees that last upper bound on ξ holds provided

$$-2x+\left[\frac{\lambda^2\|W\|^2\tau^2}{2}\right]^2<-2\lambda^2\cosh(\|W\|\tau)+\lambda^8\cosh^2(\|W\|\tau). \tag{62}$$

By using the explicit formula

$$x=\frac{\lambda^2\tau^2}{2(1+\mathrm{e}^{-\beta E_{\mathscr{E}}})}\left(\alpha_1+\alpha_2+(1+\mathrm{e}^{-\beta E_{\mathscr{E}}})|a-d|^2\mathrm{sinc}^2\left(\frac{\tau E_{\mathscr{E}}}{2}\right)\right),$$

one easily verifies that (62) holds provided that $|\lambda|<\lambda_0$. □

Proof of Theorem 11. We just have to show that

$$\mathrm{p}\big(M(\omega)\in\mathscr{M}_{(E)}\big)>0. \tag{63}$$

We consider condition 1 only, condition 2 is dealt with in the same way. Due to assumption (S3), there is a set $\Omega_0\subset\Omega$, s.t. $\mathrm{p}(\Omega_0)>0$, and, for all $\omega\in\Omega_0$, we have $\sin^2(\tau(\omega)(E_{\mathscr{E}}-E_{\mathscr{S}})/2)\geq\sin^2(\eta_-)$ and $\tau(\omega)\geq 2\eta_-|E_{\mathscr{E}}-E_{\mathscr{S}}|^{-1}$. Due to Lemma 10, we have that $M(\omega)\in\mathscr{M}_{(E)}$ provided λ^2 satisfies the bounds given in point 1 of Theorem 11, and this for any $\omega\in\Omega_0$. Thus (63) holds. □

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String-Localized Quantum Fields, Modular Localization, and Gauge Theories

Jens Mund*

Abstract The concept of modular localization introduced by Brunetti, Guido and Longo, and Schroer, can be used to construct quantum fields. It combines Wigner's particle concept with the Tomita-Takesaki modular theory of operator algebras. I report on the construction of free fields which are localized in semi-infinite strings extending to space-like infinity (mainly in collaboration with B. Schroer and J. Yngvason). Particular applications are: The first local (in the above sense) construction of fields for Wigner's massless "infinite spin" particles; String-localized vector/tensor potentials for Photons and Gravitons, respectively; Massive vector bosons. Some speculative ideas are be presented concerning the perturbative construction of gauge theories (and quantum gravity) completely within a Hilbert space, trading gauge dependence with dependence on the direction of the localization string.

1 The Notion of String-Localized Quantum Fields

The principle of locality demands that observables be measurable in bounded regions of spacetime, and that observables localized in space-like separated regions be compatible. This principle is usually implemented by (point-like localized) quantum fields which commute for space-like separated arguments. In addition to the observables there may be, however, unobservable charge–carrying fields. In models, these are constructed first and then the observables are constructed from them, usually selected by a global gauge principle. (For example, the observables in the case of a charged scalar field $\varphi(x)$ are generated by the currents $j_\mu(x)$.)

Jens Mund
Departamento de Física, ICE, Univ. Federal de Juiz de Fora (UFJF), Juiz de Fora, Brazil, e-mail: mund@fisica.ufjf.br

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The unobservable fields need, in general, not be localized in bounded regions. In some cases, the fundamental fields even *cannot be localized* in bounded regions: For example, if they carry a so-called "gauge charge" [8], that is a charge which can be determined at space-like infinity by a version of Gauss' law. Another instance are fields whose basic excitations are certain "exotic" particle types, namely Anyons [35] in $2+1$ dimensions and Wigner's so-called massless "infinite spin" particles [34]. The former correspond to irreducible massive positive-energy representations of the Poincaré group whose spin is not integer or half-integer (which is admitted in two space dimensions). The work of Doplicher et al. [11] implies that the corresponding fields cannot be compactly localized. The latter correspond to irreducible massless representations with infinitely many polarization degrees of freedom, corresponding to a faithful representation of the little group $E(2)$. J. Yngvason has shown [36] that fields with such excitations cannot be point-like localized in the sense of Wightman fields.

Besides the necessity to introduce "non-local" fields in certain models, an important motivation to consider such fields is that they promise better UV behaviour and hence a larger class of renormalizable interactions. In fact, this has been the motivation in the 50^{ies} to study "non-local interactions" [17, 20], but this hope has been disappointed in the 70^{ies} [19]. From the present point of view, the reason was that in these days there has not been known a proper notion of "non-locality". Namely, the charge carrying fields do have to satisfy *some* localization properties since they must generate local observables. This has not been achieved in the mentioned approaches [19].

Later, it has been realized that a proper notion of "non-locality" is localizability in *space-like cones* [18, 9]. A space-like cone is a salient cone in space-time which extends to space-like infinity. In particular, it has been shown by Buchholz and Fredenhagen [9] that if the theory is purely massive and allows for the construction of local observables, then the charged fields must be localized[2] in space-like cones.

Important structural results have been shown for theories with such localization, like the construction of scattering states [9], analyticity of the S-matrix [3], the analysis of the superselection charge structure [10], and the Bisognano-Wichmann and PCT theorems [21]. Similarly, Brunetti et al. [7] have shown the existence of a free field algebra localized in space-like cones for all (bosonic) particle types, including the massless "infinite spin" particles.

Steinmann [27], inspired by the ideas of Mandelstam [18], introduced the notion of quantum fields localized on *space-like strings*, idealizing a cone. Such "string" is a ray extending from a point in Minkowski space to infinity in some space-like direction. More precisely, if x is a point in $\mathbb{R}^4$ and e is a point in the manifold of space-like directions,

$$H := \{e \in \mathbb{R}^4, e \cdot e = -1\}, \tag{1}$$

then the string $S_{x,e}$ emanating from x in direction e is given by

[2] In the case of charged fields, localization means that space-like separated fields have vanishing commutators or anti-commutators or, in $2+1$ dimensions, satisfy more general (braided) commutation relations.

$$S_{x,e} := x + \mathbb{R}_0^+ e. \tag{2}$$

Steinmann proved the Jost-Schroer theorem for fields with such localization [27]. In [24, 25], we have elaborated on this concept, introducing the notion of a covariant string-localized quantum field, as follows.

Definition 1. A covariant *string-localized quantum field* is an operator valued distribution $\varphi(x, e)$ on $\mathbb{R}^4 \times H$ satisfying

(i) String-locality: If $S(x, e)$ and $S(x', e')$ are space-like separated, then

$$[\varphi(x, e), \varphi(x', e')] = 0; \tag{3}$$

(ii) Covariance: There is a representation U of the Poincaré group $\mathscr{P}_+^\uparrow$ such that

$$U(a, \Lambda)\varphi(x, e)U(a, \Lambda)^{-1} = \varphi(\Lambda x + a, \Lambda e) \tag{4}$$

holds for all $(a, \Lambda) \in \mathscr{P}_+^\uparrow$.

(We also consider the case where the fields have, in addition, tensor or spinor indices, cf. below.) Our original aim, motivating the introduction of this concept, was an explicit construction of free fields for the massless infinite spin particles, improving the existence result of Brunetti et al. [7]. This goal has been reached [24, 25], but we also constructed free covariant string-localized fields for all other particle types. These by-products turned out to be at least as interesting than the original objective, since these fields might be a good starting point for a perturbative construction of new interacting quantum fields, as I shall try to motivate in Sect. 4.

The next section is meant to sketch the role of modular localization in our construction of free fields. Section 3 summarizes results on free fields and their (time-ordered) two-point functions, and Sect. 4 gives a speculative outlook on the construction of interacting string-localized fields.

2 Modular Localization and the Construction of Free String-Localized Fields

In the point-localized case, covariance of free fields essentially already (almost) implies locality. In the string-localized case, this is not so and there are no guidelines from the usual field theory methods in implementing locality (3). Hence independent ideas are warranted. In the context of algebraic QFT, there is an appropriate concept, the so-called *modular localization*. This concept has been introduced by Brunetti et al. [7] and by Schroer [14]. It is based on the Bisognano-Wichmann theorem [2, 21], which asserts that for a large class of models, certain algebraic invariants of the field algebra are fixed by the (ray) representation of the Poincaré group under which the field transforms, and the S-matrix. These algebraic invariants are the Tomita operators $S(\mathscr{O})$ of the algebra of fields localized in $\mathscr{O}$, for each space-time region $\mathscr{O}$.

The principle of modular localization consists in inverting the argument: Namely, the Tomita operators can be consistently constructed from the representation of the Poincaré group (and the S-matrix). This has been done by the author for Anyons in $d = 2 + 1$ at the single particle level [22]. Moreover, (in the non-Anyon case) the family of Tomita operators allows for the construction of free local fields. This concept of modular localization has been used by Brunetti et al. in the mentioned existence proof of free fields localized in space-like cones for every bosonic particle type, including the massless infinite spin particles [7].

As mentioned, the aim of [24, 25] was to achieve more, namely an explicit construction, and idealization of the space-like cones to strings $S_{x,e}$. By the Jost-Schroer theorem for string-localized fields [27], it suffices to solve the problem on the level of the single particle space, consisting of L^2 functions on the mass shell H_m^+ with values in the "little Hilbert space" (corresponding to the spin degrees of freedom). The field $\varphi(x, e)$ must create from the vacuum Ω a single particle state of the form

$$\langle p \,|\, \varphi(x, e)\Omega \rangle = e^{ipx} u(e, p), \quad p \in H_m^+, \tag{5}$$

where $u(e, p)$ is a distribution in $e \in H$ and a function in $p \in H_m^+$ with values in the "little Hilbert space" satisfying certain properties which encode locality and covariance: Firstly, our requirement of string-locality (3) implies that $\varphi(x, e)\Omega$ is (after smearing) in the domain of definition of each Tomita operator pertaining to any space-like cone containing the string $S_{x,e}$. The concept of modular localization then implies that for fixed p, $u(e, p)$ is the boundary value of an analytic function on the tuboid $\mathscr{T}_+$ in the natural complexification of H consisting of those complex e whose imaginary part is in the open forward light cone. This function is of moderate growth near the real "boundary" H, in the sense of [4], thereby defining $u(e, p)$ as a distribution on H. Secondly, covariance (4) implies that u satisfies the *intertwiner property*

$$D(R(\Lambda, p))u(\Lambda^{-1}e, \Lambda^{-1}p) = u(e, p) \tag{6}$$

for $(e, p) \in \mathscr{T}_+ \times H_m^+$ and $\Lambda \in \mathscr{L}_+^\uparrow$. Here, $R(\Lambda, p)$ is the Wigner rotation and D is the representation of the little group which induces the irreducible (ray) representation of the Poincaré group corresponding to the particle type at hand. With the intertwiner function $u(e, p)$ one associates a Hermitean field acting in the Fock space over the corresponding one particle space, via

$$\varphi(x, e) = \int_{H_m^+} d\mu(p) \big\{ e^{ip\cdot x} u(e, p) \circ a^*(p) + e^{-ip\cdot x} \overline{u(e, p)} \circ a(p) \big\}. \tag{7}$$

Here, $d\mu(p)$ is the Lorentz invariant measure on H_m^+, and the circle $\circ$ denotes (sloppily speaking) summation/integration over the spin degrees of freedom. (In (7) it has been assumed that $u(e, p)$ satisfies a certain self-conjugacy property (which can be achieved for all particle types), yielding a Hermitean field.) This field is then in fact covariant in the sense of (4) under the second quantization U of the corresponding irreducible representation, and string-localized in the sense of (3).

3 Results on Free String-Localized Fields

Along the indicated lines, we have constructed free covariant string-localized fields for all bosonic particle types, including the massless infinite spin particles in [25]. (String-localized fermions can also be constructed; they need an additional spinor index.) Our fields satisfy the Reeh-Schlieder and Bisognano-Wichmann properties.

We have also found the following uniqueness result. Every covariant string-localized field is of the form (7), and the intertwiner function u is unique up to multiplication with a function of $e \cdot p$ which is meromorphic on the upper complex half plane. (That is to say, if $\hat{u}$ is another intertwiner function, then $u(e, p) = F(e \cdot p)\hat{u}(e, p)$, where F is a numerical function, meromorphic on the complex upper half plane.)

Due to the worse localization, our fields have a better short distance behaviour than their point-like localized counterparts in the cases where these exist. For example, for massless particles with helicity ± 1 and ± 2, corresponding to photons and gravitons, the Fourier transforms of the propagators[3] behave like $|p|^{-2}$ for large p, cf. (12), (17) and (22) below. This behaviour is a prerequisite for any non-trivial interaction, and can in the point-localized case be achieved only in the setting of gauge theory, at the price of an indefinite metric space or loss of covariance. For massive particles of arbitrary spin s we also have constructed fields whose propagators behave like $|p|^{2s-2-2\alpha}$, where α is a positive number smaller than 2. This is to be contrasted with the point-localized case, where the propagators for spin s behave at best like $|p|^{2s-2}$ [32].

In the following we present some details on the fields, two-point functions and propagators for the particular models. More details, and the proofs, shall be published in a forthcoming paper [23].

3.1 Fields and Two-Point Functions

Let us now specify the fields and/or two-point functions for the particular cases: Massless infinite spin particles, photons, massive vector bosons, massive fields with arbitrary spin without vector/tensor indices, and massless fields with helicity ± 2.

Massless Infinite Spin Particles

These correspond to representations of the Poincaré group where the inducing representation of the little group $E(2) = \mathbb{R}^2 \rtimes SO(2)$, corresponding to the spin degrees of freedom, is faithful. Such inducing representation D_κ is infinite dimensional, characterized by a parameter $\kappa > 0$, and acts on $L^2(\mathbb{R}^2, \delta(k^2 - \kappa^2)d^2k)$ as

[3] By (Feynman) propagator, we mean time-ordered two-point function.

$$(D_\kappa(c, R)\psi)(k) := e^{ic\cdot k}\psi(R^{-1}k),$$

$(c, R) \in \mathbb{R}^2 \rtimes SO(2)$. For these particles, we have found intertwiner functions u^α characterized by a real parameter $\alpha > 0$:

$$u^\alpha(e, p)(k) = e^{i\pi\alpha/2} \int d^2c e^{ic\cdot k}(B_p \Lambda_c \xi \cdot e)^{-\alpha}, \tag{8}$$

where B_p is a boost which maps a fixed base point in H_0^+ to p, Λ_c is the Lorentz transformation corresponding to a c–translation in the stability group $E(2)$ of the base point, and ξ is a lightlike vector invariant under the rotation subgroup of the $E(2)$. This intertwiner function gives rise, via (7), to a quantum field which satisfies all requirements from Definition 1.

The problem which has thus been solved has already been posed by Wigner [34] and has resisted considerable efforts of several generations of elementary particle physicists [36, 16, 34, 1]. (In the mentioned articles, covariant fields have been constructed, but the issue of localization has not been solved.)

Vector Potentials for Photons

For massless particles with finite helicity (i.e. finite-dimensional representation of the little group) the fields must carry a vector index, in addition to the string direction e. For photons, we constructed a string-localized vector boson $A_\mu(x, e)$, acting in the physical photon Hilbert space (the second quantization of the direct sum of irreducible representation spaces for helicity 1 and -1). It transforms as

$$U(a, \Lambda)A_\mu(x, e)U(a, \Lambda)^{-1} = A_\nu(a + \Lambda x, \Lambda e)\Lambda^\nu{}_\mu \tag{9}$$

and satisfies string-locality in the sense of (3). It is indeed a vector potential for the field strength $F_{\mu\nu}$ (the unique free Wightman field corresponding to the electromagnetic field strength and acting in the mentioned Hilbert space) in the sense that its exterior derivative dA (w.r.t. x) coincides with F, i.e. $F_{\mu\nu}(x) = \partial_\mu A_\nu(x, e) - \partial_\nu A_\mu(x, e)$. It also satisfies the Lorentz and axial "gauge" conditions

$$\partial^\mu A_\mu(x, e) = 0, \qquad e^\mu A_\mu(x, e) = 0. \tag{10}$$

However, these conditions are satisfied by *every* free vector field $A_\mu(x, e)$ for photons acting in the physical Hilbert space and transforming as in (9); hence they cannot be regarded as additional gauge conditions in this context. Our vector potential is completely fixed by the requirements of string-locality (3), covariance (9) and that its exterior derivative is independent of e [25, Proposition 5.1]. (The latter requirement is analogous to gauge independence in the usual formulation. It implies that dA coincides with the electromagnetic field strength [25, Proof of Proposition 5.1].) It is built as in (7) from the following intertwiner function:

$$u(e,p)_{\pm,\mu} = \lim_{\varepsilon\to 0} \frac{\hat{e}_\pm(p)\cdot e}{e\cdot p + i\varepsilon} p_\mu - \hat{e}_\pm(p)_\mu. \tag{11}$$

Here, $\hat{e}_\pm(p)$ are the polarization vectors $\hat{e}_\pm(p) := B_p\hat{e}_\pm$ where $\hat{e}_\pm := 2^{-1/2}(0,1,\mp i,0)$ and B_p is the mentioned boost which maps $(1,0,0,1)$ to p. The ε-prescription of the expression $(e\cdot p+i\varepsilon)^{-1}$ in (11) is meant as follows: For fixed p, first integrate over a test function in e, then take the limit $\varepsilon\to 0$. (Since $e\cdot p$ has positive imaginary part for $p\in H_0^+$ and e in the mentioned tuboid $\mathscr{T}_+$, this prescription corresponds precisely to the one indicated above, before (6).) The result is bounded [23] by $|p|^{-1}$ times a seminorm of the test function, where $|\cdot|$ is any norm on $\mathbb{R}^4$. This holds not only for $p\in H_0^+$, but for all $p\in\mathbb{R}^4$ (which is relevant in the analysis of the propagator).

The two-point function of the corresponding field is given by

$$\begin{aligned}(\Omega, A_\mu(x,e)A_\nu(x',e')\Omega) &= \int_{H_0^+} d\mu(p) e^{ip\cdot(x'-x)} M_{\mu\nu}(p;e,e'),\\ M_{\mu\nu}(p;e,e') &\doteq -g_{\mu\nu} - \frac{p_\mu p_\nu (e\cdot e')}{(e\cdot p - i\varepsilon)(e'\cdot p + i\varepsilon')}\\ &\quad + \frac{e_\nu p_\mu}{e\cdot p - i\varepsilon} + \frac{e'_\mu p_\nu}{e'\cdot p + i\varepsilon'}.\end{aligned} \tag{12}$$

Recall that in the quantization of the *point-like* localized vector potential, one has the freedom of a choice of gauge, with the following two alternatives: A covariant gauge only exists in an indefinite metric space [28]. In a Hilbert space representation, there are only non-covariant gauges, among them the axial gauge $e^\mu A_\mu(x,e)=0$ where e is a *fixed* direction. In this gauge, the two-point function has the same form as in (12) (with $e=e'$), with two significant disadvantages compared with our string-localized fields: Firstly, it is not Poincaré invariant since e is fixed; and secondly, there is no convincing regularization of the singularities $e\cdot p$ [33]. (In our approach, the factors $(e\cdot p+i\varepsilon)^{-1}$ are regular after smearing with a test function in e, and this regularization is fixed by the same requirements as the field $A_\mu(x,e)$ itself.)

Massive Vector Bosons

There is also a string-localized field for massive vector bosons with spin one [23]. As in the above massless case, it is fixed by the requirements of covariance (9), string-locality and that $dA(x,e)$ be independent of e. It has the same two-point function as the massless (photon) counterpart, cf. (12), except that it is concentrated on the positive mass shell H_m^+, where $m>0$ is the respective mass. This interesting fact might allow for a treatment of the infrared problem (adiabatic limit) in perturbative QED by starting from massive QED and letting $m\to 0$. The massive analogue of (12) implies that the propagator of our string-localized massive vector boson behaves like $|p|^{-2}$ for large momenta. This is worthwile comparing with the point-like localized counterpart, whose propagator contains a term $\sim |p|^0$, which excludes

any interesting interactions (unless one adds ghost degrees of freedom and uses an indefinite metric representation, in which case a $|p|^{-2}$ behaviour can be achieved).

Massive Bosonic Particles with Arbitrary Spin

For particles with mass m and arbitrary spin $s \in \mathbb{N}_0$ we have fields $\varphi(x, e)$ without vector or tensor indices, as in (7). The corresponding single particle space consists of functions from the positive mass shell H_m^+ into the little Hilbert space $\mathbb{C}^{2s+1}$. Our intertwiner functions are characterized by a positive real number $\alpha > 0$, and are given by [25]

$$u(e, p)_k := i^\alpha u_0 (A_p^{-1} e)_k (e \cdot p + i\varepsilon)^{-\alpha}, \quad k = -s, \ldots, s, \tag{13}$$

$$u_0(e)_k := i^s (1 + (e^0)^2)^{s/2} \overline{Y_{s,k}(n(e))}. \tag{14}$$

Here, A_p is a boost which maps the reference momentum $(m, 0, 0, 0)$ to p, $Y_{s,k}$ are the spherical harmonics, and $n(e) := (1 + (e^0)^2)^{-1/2}(e^1, e^2, e^3) \in S^2$. For $s = 1$, the corresponding two-point function comes out as

$$(\Omega, \varphi(x, e)\varphi(x', e')\Omega) = \text{const.} \int_{H_m^+} d\mu(p) e^{ip\cdot(x'-x)} \frac{(e \cdot p)(e' \cdot p) - m^2(e \cdot e')}{(e \cdot p - i\varepsilon)^\alpha (e' \cdot p + i\varepsilon')^\alpha}. \tag{15}$$

For $s \neq 1$, the numerator in (15) is replaced by a polynomial in $e \cdot p$, $e' \cdot p$ and $e \cdot e'$ of degree s. As indicated above, the distribution $t_p^\alpha(e) := (e \cdot p + i\varepsilon)^{-\alpha}$, after integrating against a testfunction in e, is bounded by $|p|^{-\alpha}$. Since $|p| > m$ for $p \in H_m^+$, it is bounded uniformly in $p \in H_m^+$ for any $\alpha > 0$. Hence at this point α may be taken as large as one wants, yielding an arbitrarily good UV behaviour. However, as motivated in Sect. 3.2, one apparently has to consider the restrictions in e of our fields to space-like hypersurfaces $\Sigma \subset H$. Now such restriction of t_p^α exists and is bounded by $|\boldsymbol{p}|^{-\alpha}$ after smearing, where $\boldsymbol{p}$ is the spatial part of p in the reference system corresponding to Σ [23]. This requires $\alpha < 3/2$.

Tensor Potentials for Linearized Gravitons

For massless particles with helicity ± 2, there is a string-localized tensor field $h_{\mu\nu}(x, e)$ transforming as a "string-tensor", similar to (9) [23]. It is a "potential" for the quantized (point-localized) free, i.e. linearized, Riemann tensor $R_{\mu\nu\alpha\beta}$ [26], in the sense that it has the classical relation with the linearized Riemann tensor:

$$R_{\mu\nu\alpha\beta}(x) = \frac{1}{2}\big\{\partial_\mu\partial_\alpha h_{\nu\beta}(x, e) + \partial_\nu\partial_\beta h_{\mu\alpha}(x, e) - \partial_\nu\partial_\alpha h_{\mu\beta}(x, e) - \partial_\mu\partial_\beta h_{\nu\alpha}(x, e)\big\}. \tag{16}$$

It is well-known that for point-localized fields these conditions cannot be satisfied in a Hilbert space representation with positive energy [29]. The two-point function of our $h_{\mu\nu}$ is given by [23]

$$\begin{aligned}(\Omega, h_{\mu\alpha}(x,e)h_{\mu'\alpha'}(x',e')\Omega) &= \int_{H_0^+} d\mu(p) e^{ip\cdot(x'-x)} M_{\mu\alpha,\mu'\alpha'}(p;e,e'),\\ M_{\mu\alpha,\mu'\alpha'}(p;e,e') &\doteq M^R_{\mu\nu\alpha\beta,\mu'\nu'\alpha'\beta'}(p)\frac{e^\nu e^\beta (e')^{\nu'}(e')^{\beta'}}{(e\cdot p - i\varepsilon)^2(e'\cdot p + i\varepsilon')^2}.\end{aligned} \tag{17}$$

Here $M^R_{\mu\nu\alpha\beta,\mu'\nu'\alpha'\beta'}(p)$ is the on-shell two-point function of the free Riemann tensor, which is a homogeneous polynomial in p of degree four, cf. [31]. Consequently, the Fourier transform of the propagator goes like $|p|^{-2}$ for large p. (It is also regular for finite p since, as mentioned above, it is being considered as a distribution in e, e' so that the factors $(e\cdot p \pm i0)^{-1}$ do not cause singularities other than $|p|^{-1}$).

3.2 Feynman Propagators

One of the perturbative construction schemes of interacting fields rests on the concept of time-ordered products of fields, the basic building blocks being time-ordered two-point functions, or Feynman propagators. In the case at hand, the string localization has to be taken into account. Given two strings $S_{x,e}$ and $S_{x',e'}$ we say that $S_{x,e}$ is *later* than $S_{x',e'}$, denoted as

$$S_{x,e} > S_{x',e'}, \tag{18}$$

iff there is a space-like hyperplane Σ of Minkowski space such that $S_{x,e}$ is in the future and $S_{x',e'}$ is in the past of Σ. We say that two strings S_1, S_2 are *comparable* if one of them is later than the other (i.e., if there they are separated by some space-like hyperplane). Note that a string is both later and earlier than another string if and only if the two strings are space-like separated. The Feynman propagators $T(x,e;x',e')$ are distributions related to the two-point functions $W(x,e;x',e') := (\Omega, \varphi(x,e)\varphi(x',e')\Omega)$ by the requirement

$$T(x,e;x',e') = \begin{cases} W(x,e;x',e'), & \text{if } S_{x,e} > S_{x',e'},\\ W(x',e';x,e), & \text{if } S_{x',e'} > S_{x,e}.\end{cases} \tag{19}$$

A complication arises from the fact that the set of points $(x,e;x',e')$ such that $S_{x,e}$ and $S_{x',e'}$ are *not* comparable contains an *open* set in $(\mathbb{R}^4 \times H)^{\times 2}$. This implies that the propagator cannot be fixed by the time-ordering requirement (19) (neither by a finite number of renormalization conditions.) A way out is to consider the restriction of T to space-like hypersurfaces of the form

$$\Sigma_u := u^\perp \cap H, \tag{20}$$

where u is a time-like unit vector. (These are the totally geodesic space-like hypersurfaces.) Namely, two strings $S_{x,e}$ and $S_{x',e'}$ with (e, e') in some Σ_u are not comparable only if they intersect [23]. We are thus led to the following definition. The *Feynman propagator* of a string-localized quantum field is a Poincaré invariant symmetric distribution T on $(\mathbb{R}^4 \times H)^{\times 2}$ whose restriction to $(\mathbb{R}^4 \times \Sigma_u)^{\times 2}$ exists for any time-like vector u and satisfies time-ordering (19). To discuss its uniqueness in concrete models, one has to determine its scaling degrees with respect to the submanifold [5] of non-comparable pairs of strings, and w.r.t. the origin $x = x' = 0$, and compare them with the respective co-dimensions.

We have found [23] Feynman propagators of our string-localized fields describing photons and massive vector bosons (12), massive particles of arbitrary spin (15) and the massless spin-2 particles (17). Namely, writing the two-point functions of these fields in the form

$$W_{\sigma,\sigma'}(x, e; x', e') = \int_{H_m^+} d\mu(p) e^{ip\cdot(x'-x)} M_{\sigma,\sigma'}(p; e, e'), \tag{21}$$

where σ, σ' are possible vector or tensor indices, the corresponding Feynman propagator is given by

$$T_{\sigma,\sigma'}(x, e; x', e') := \frac{i}{2\pi} \int d^4p e^{ip\cdot(x'-x)} \frac{M_{\sigma,\sigma'}(p, e, e')}{p^2 - m^2 + i0}. \tag{22}$$

(In the massive case with arbitrary spin (15), this distribution is well-defined iff the positive number α is smaller than two, and the restriction to Σ_u exists if α is smaller than $3/2$. In the other cases, the restrictions exist without further requirements.) Uniqueness of our propagators shall be discussed in a forthcoming paper [23].

4 Outlook: Interacting String-Localized Fields

The specific properties of our string-localized free fields raise the hope that they should be a good starting point for a perturbative construction of interacting string-localized fields. In contrast to the case of point-localized fields, the various construction schemes are not equivalent in the case at hand. For example, the Yang-Feldman approach does not seem to work for string-localized fields, for reasons similar to the ones found already in the 70's in the context of "non-local" interactions [19]: The (string-) localization is lost in higher orders. But there is one perturbative scheme which seems to work for string-localized fields: The so-called causal construction of Epstein and Glaser [13], based on ideas of Stueckelberg and Bogoliubov.

We shall briefly sketch this approach (see [5, 26] for a detailed account). One starts with a free field φ or a set of basic free fields acting in a Hilbert space, and an "interaction Lagrangean" $\mathscr{L}_I$. This is a Wick polynomial in the free fields, interpreted as the first order of the S-matrix. (However, a Lagrangean formulation of the theory is not necessary [30]). The interaction Lagrangean determines a specific class

of Wick polynomials, namely its derivatives w.r.t. the basic fields. For Wick polynomials W_i in this class, one defines time-ordered products $T W_1(x_1) \cdots W_n(x_n)$ recursively, requiring that

$$T W_1(x_1) \cdots W_n(x_n) = T W_1(x_1) \cdots W_k(x_k) T W_{k+1}(x_{k+1}) \cdots W_n(x_n) \tag{23}$$

if all of the events $x_1, \ldots, x_k$ are later than the events $x_{k+1}, \ldots, x_n$ in some reference frame. Together with (translational) covariance, this fixes the time-ordered products up to the point $x_1 = \cdots = x_n = 0$. (Re-) normalization then consists in the extension into this point. Having constructed the time-ordered products, one defines Bogoliubov's S-Matrix, depending on a test function of compact support g and a Wick polynomial W in the mentioned class, as the formal series

$$S(gW) := \sum_{n=0}^{\infty} \frac{i^n}{n!} \int dx_1 \cdots dx_n g(x_1) \cdots g(x_n) T W(x_1) \cdots W(x_n). \tag{24}$$

The interpretation of $S(g\mathscr{L}_I)$ is that it formally constitutes the S-matrix for the Hamiltonian

$$H_I(t) \doteq - \int d^3\mathbf{x} \mathscr{L}_I(t, \mathbf{x}) g(t, \mathbf{x})$$

in the interaction picture. (The infrared problem consists in the so-called adiabatic limit, $g \to$ const.) One then defines for every free field φ an interacting field φ_I via Bogoliubov's formula:

$$\varphi_I(f) := \frac{1}{i} \frac{d}{d\lambda} S(g\mathscr{L}_I)^{-1} S(g\mathscr{L}_I + \lambda f \varphi)|_{\lambda=0}. \tag{25}$$

Due to the time-ordering prescription (23), the S-matrix satisfies the so-called causal factorization property which in turn implies locality of the interacting fields.

This scheme might be transferred to the string-localized case as follows. The time-ordering prescription of string-localized Wick products $W(x, e)$ must take the strings $S_{x,e}$ into account: (23), with (x_i, e_i) instead of x_i, must hold if all strings $S_{x_1,e_1}, \ldots, S_{x_k,e_k}$ are later than the strings $S_{x_{k+1},e_{k+1}}, \ldots, S_{x_n,e_n}$ in the sense of (18). Bogoliubov's S-matrix then depends on test functions $g(x, e)$ living on $\mathbb{R}^4 \times H$, and the multiple integral in (24) extends also over $H^{\times n}$. $S(g\mathscr{L}_I)$ is then the formal S-matrix for the interaction Hamiltonian

$$H_I(t) \doteq - \int_{x^0=t} d^3\mathbf{x} \int_H d\sigma(e) \mathscr{L}_I(x, e) g(x, e)$$

in the interaction picture, where $d\sigma(e)$ denotes the Lorentz invariant measure on H. The interacting fields are defined as in (25), with f a test function on $\mathbb{R}^4 \times H$. As in the point-localized case, the time-ordering prescription implies a causal factorization property of the S-matrix which in turn implies *string-locality* of the interacting fields in the sense of (3).

For the reason indicated in Sect. 3.2, it appears necessary to restrict the time-ordered products to space-like hyperplanes Σ_u of the form (20). Then Bogoliubov's S-matrix and the interacting fields depend on the time-like vector u. A possible mechanism to achieve independence of this vector, and at the same time admit the construction of *local* (i.e., e-independent and point-localized) observables, is to imitate gauge theories, with "gauge dependence" being replaced by "dependence on the string e". Consider, for example, the massless or massive vector boson $A_\mu(x, e)$. Since the exterior derivative is independent of e, $A_\mu(x, e)$ and $A_\mu(x, e')$ differ by the derivative of a field $\Phi(x, e, e')$. (In contrast to the gauge theory case, this field is in the algebra of the A_μ's, and needs no new degrees of freedom.) Therefore, if we take the interaction Lagrangean $\mathscr{L}_I(x, e) = :j^\mu(x)A_\mu(x, e):$, where j^μ is the conserved current of a charged field, we have

$$\mathscr{L}_I(x, e') = \mathscr{L}_I(x, e) + i\partial_\mu W^\mu(x; e, e') \tag{26}$$

in the sense of bi-distributions. This implies that Bogoliubov's S-matrix $S(g\mathscr{L}_I)$ is independent of the time-like vector u and of the string e at first order, in the adiabatic limit $g \to$ const. Independence[4] at higher orders then amounts to a (re-) normalization condition on the time-ordered products analogous to the "perturbative gauge invariance" [26]. If this e-independence of the S-matrix in the adiabatic limit can be implemented, then the interacting counterpart $\varphi_I(x)$ of any free field $\varphi(x)$ which does not depend on e also does not depend on e and is point-like localized. This holds in particular for the fields $F_I^{\mu\nu}(x)$, where $F = dA$, and $j_I^\mu(x)$. These fields will then generate an observable algebra with point-like localization.

We conclude with some speculative remarks on possible models based on this construction. As indicated, the construction should be attempted to carry through for QED, and for massive vector bosons. A more speculative possible application is the perturbative construction of quantum gravity along rather conservative lines. Such construction would start from a family of string-localized free tensor potentials $h_{\mu\nu}(x, e)$ as described above, one for each background metric within a certain class of space-times. Here, (x, e) is a point in the tangent bundle of the space-time, and the string $S_{x,e}$ should be defined as the semi-infinite geodesic curve starting from x in the direction $e \in T_xM$. Each $h_{\mu\nu}$ would describe the quantum fluctuations around the given classical background. As interaction Lagrangean $\mathscr{L}_I$ one would take the (e-dependent analogue of the) usual corresponding part of the Einstein-Hilbert Lagrangean. The family of resulting interacting fields for every background should be constructed in such a way that a change of background metric amounts to a symmetry of the theory, in the sense explained by Brunetti and Fredenhagen in [6]. As explained there, this would implement independence of the gravitational background.

It is also possible that the proposed scheme allows for the perturbative construction of non-Abelian gauge theory analogues, and that it might even admit (renormal-

[4] Independence of u and e means that the nth term in the expansion (24) of $S_u(g \otimes h\mathscr{L}_I)$, $g \otimes h \in \mathscr{D}(\mathbb{R}^4 \times H)$, factorizes as $(\int_{\Sigma_u} hd\sigma)^n$ times an operator $S^{(n)}$ which is independent of h and u. The limit $h \to 1$ then exists and yields a factor $(4\pi)^n$, independent of u.

izable) interactions which are not admitted in the gauge theory setting. For example, one might speculate that there is a string-localized model with self-interacting vector bosons without a Higgs particle. (In the point-localized case, such model would either violate unitarity or renormalizability [15].) Apart from possible new models, there is an esthetic motivation for these constructions, namely: In the gauge theoretic approach, the construction detours through a huge realm of unphysical quantities (ghosts and an indefinite metric space), which one would like to avoid, following Ockham's razor. Our approach, on the other hand, works completely in Hilbert space and does not need ghosts (this is in accord with the well-known fact that in the axial gauge the ghosts decouple).

If these constructions work, it would be interesting to discuss the following question. The work of Scharf et al. [12] show that the principles of gauge invariance (of the observable quantities) and renormalizability fix, to a great extent, the possible interactions for a given set of particle types. The question is if the same holds in our approach, where gauge invariance is replaced by independence of the string directions e. Since this independence is equivalent with point-like localization, this would ultimately mean the following: The principles of *locality* and renormalizability fix the possible interactions. This would be very satisfying, since these principles are, in contrast to the gauge principle, intrinsic to quantum field theory.

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Kinks and Particles in Non-integrable Quantum Field Theories

Giuseppe Mussardo

Abstract In this talk we discuss an elementary derivation of the semi-classical spectrum of neutral particles in two field theories with kink excitations. We also show that, in the non-integrable cases, each vacuum state cannot generically support more than two stable particles, since all other neutral excitations are resonances, which will eventually decay.

1 Introduction

Two-dimensional massive Integrable Quantum Field Theories (IQFTs) have proven to be one of the most successful topics of relativistic field theory, with a large variety of applications to statistical mechanical models. The main reason for this success consists of their simplified on-shell dynamics which is encoded into a set of elastic and factorized scattering amplitudes of their massive particles [33, 31]. The two-particle S-matrix has a very simple analytic structure, with only poles in the physical strip, and it can be computed combining the standard requirements of unitarity, crossing and factorization together with specific symmetry properties of the theory. The complete mass spectrum is obtained looking at the pole singularities of the S-matrix elements. Off-mass shell quantities, such as the correlation functions, can be also determined once the elastic S-matrix and the mass spectrum are known. In fact, one can compute the exact matrix elements of the (semi)local fields on the asymptotic states with the Form Factor (FF) approach [29, 20], and use them to write down the spectral representation of the correlators. By following this approach, it has been possible, for instance, to tackle successfully the long-standing problem of spelling out the mass spectrum and the correlation functions of the two dimensional Ising

Giuseppe Mussardo
International School for Advanced Studies, Via Beirut 1, 34013 Trieste, Italy and Istituto Nazionale di Fisica Nucleare, Sezione di Trieste, Trieste, Italy, e-mail: mussardo@sissa.it

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model in a magnetic field [31, 8, 10], as well as many other interesting problems of statistical physics (for a partial list of them see, for instance, [23]).

The S-matrix approach can be also constructed for massless IQFTs [32, 34, 14, 11], despite the subtleties in defining a scattering theory between massless particles in $(1+1)$ dimensions, and turns out to be useful mainly when conformal symmetry is not present. In this case, massless IQFTs generically describe the Renormalization Group trajectories connecting two different Conformal Field Theories, which respectively rule the ultraviolet and infrared limits of all physical quantities along the flows.

Given the large number of remarkable results obtained by the study of IQFTs, one of the most interesting challenges is to extend the analysis to the non-integrable field theories, at least to those obtained as deformations of the integrable ones and to develop the corresponding perturbation theory. The breaking of integrability is expected to considerably increase the difficulties of the mathematical analysis, since scattering processes are no longer elastic. Non-integrable field theories are in fact generally characterized by particle production amplitudes, resonance states and, correspondingly, decay events. All these features strongly effect the analytic structure of the scattering amplitudes, introducing a rich pattern of branch cut singularities, in addition to the pole structure associated to bound and resonance states. For massive non-integrable field theories, a convenient perturbative scheme was originally proposed in [12] and called Form Factor Perturbation Theory (FFPT), since it is based on the knowledge of the exact Form Factors (FFs) of the original integrable theory. It was shown that, even using just the first order correction of the FFPT, a great deal of information can be obtained, such as the evolution of their particle content, the variation of their masses and the change of the ground state energy. Whenever possible, universal ratios were computed and successfully compared with their value obtained by other means. Recently, for instance, it has been obtained the universal ratios relative to the decay of the particles with higher masses in the Ising model in a magnetic field, once the temperature is displayed away from the critical value [18] (see also the contribution by G. Delfino in this proceedings [7]). For other and important aspects of the Ising model along non-integrable lines see the references [22, 15, 28, 16]. Applied to the double Sine–Gordon model [9], the FFPT has been useful in clarifying the rich dynamics of this non-integrable model. In particular, in relating the confinement of the kinks in the deformed theory to the non-locality properties of the perturbed operator and predicting the existence of a Ising-like phase transition for particular ratios of the two frequencies—results which were later confirmed by a numerical study [1]. The FFPT has been also used to study the spectrum of the $O(3)$ non-linear sigma model with a topological θ term, by varying θ [3, 4].

In this talk I would like to focus the attention on a different approach to tackle some interesting non-integrable models, i.e. those two dimensional field theories with kink topological excitations. Such theories are described by a scalar real field $\varphi(x)$, with a Lagrangian density

$$\mathscr{L} = \frac{1}{2}(\partial_\mu \varphi)^2 - U(\varphi), \tag{1}$$

where the potential $U(\varphi)$ possesses several degenerate minima at $\varphi_a^{(0)}$ ($a = 1, 2, \ldots, n$), as the one shown in Fig. 1. These minima correspond to the different vacua $|a\rangle$ of the associate quantum field theory.

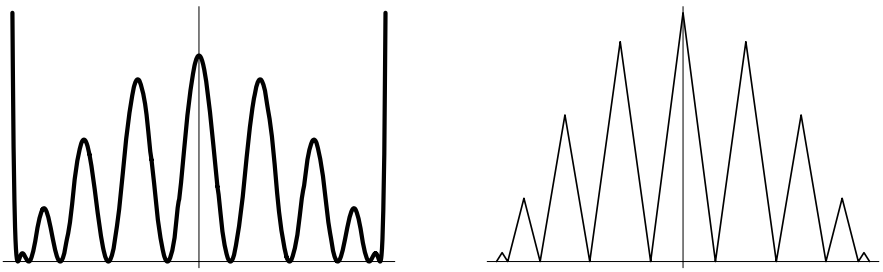

Fig. 1 Potential $U(\varphi)$ of a quantum field theory with kink excitations (A) and istogram of the masses of the kinks (B)

The basic excitations of this kind of models are kinks and anti-kinks, i.e. topological configurations which interpolate between two neighbouring vacua. Semiclassically they correspond to the static solutions of the equation of motion, i.e.

$$\partial_x^2 \varphi(x) = U'[\varphi(x)], \tag{2}$$

with boundary conditions $\varphi(-\infty) = \varphi_a^{(0)}$ and $\varphi(+\infty) = \varphi_b^{(0)}$, where $b = a \pm 1$. Denoting by $\varphi_{ab}(x)$ the solutions of this equation, their classical energy density is given by

$$\epsilon_{ab}(x) = \frac{1}{2}\left(\frac{d\varphi_{ab}}{dx}\right)^2 + U(\varphi_{ab}(x)), \tag{3}$$

and its integral provides the classical expression of the kink masses

$$M_{ab} = \int_{-\infty}^{\infty} \epsilon_{ab}(x). \tag{4}$$

It is easy to show that the classical masses of the kinks $\varphi_{ab}(x)$ are simply proportional to the heights of the potential between the two minima $\varphi_a^{(0)}$ and $\varphi_b^{(0)}$: their istogram provides a caricature of the original potential (see Fig. 1).

The classical solutions can be set in motion by a Lorentz transformation, i.e. $\varphi_{ab}(x) \to \varphi_{ab}[(x \pm vt)/\sqrt{1-v^2}]$. In the quantum theory, these configurations describe the kink states $|K_{ab}(\theta)\rangle$, where a and b are the indices of the initial and final vacuum, respectively. The quantity θ is the rapidity variable which parameterizes the relativistic dispersion relation of these excitations, i.e.

$$E = M_{ab} \cosh\theta, \qquad P = M_{ab} \sinh\theta. \tag{5}$$

Conventionally $|K_{a,a+1}(\theta)\rangle$ denotes the *kink* between the pair of vacua $\{|a\rangle, |a+1\rangle\}$ while $|K_{a+1,a}\rangle$ is the corresponding *anti-kink*. For the kink configurations it may be useful to adopt the simplified graphical form shown in Fig. 2.

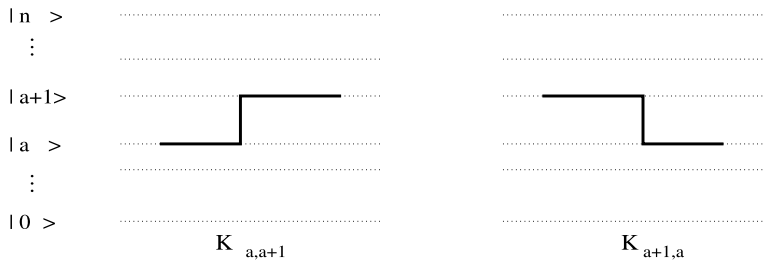

Fig. 2 Kink and antikink configurations

The multi-particle states are given by a string of these excitations, with the adjacency condition of the consecutive indices for the continuity of the field configuration

$$|K_{a_1,a_2}(\theta_1)K_{a_2,a_3}(\theta_2)K_{a_3,a_4}(\theta_3)\ldots\rangle, \quad (a_{i+1} = a_i \pm 1) \tag{6}$$

In addition to the kinks, in the quantum theory there may exist other excitations in the guise of ordinary scalar particles (breathers). These are the neutral excitations $|B_c(\theta)\rangle_a$ $(c = 1, 2, \ldots)$ around each of the vacua $|a\rangle$. For a theory based on a Lagrangian of a single real field, these states are all non-degenerate: in fact, there are no extra quantities which commute with the Hamiltonian and that can give rise to a multiplicity of them. The only exact (alias, unbroken) symmetries for a Lagrangian as (1) may be the discrete ones, like the parity transformation P, for instance, or the charge conjugation $\mathscr{C}$. However, since they are neutral excitations, they will be either even or odd eigenvectors of $\mathscr{C}$.

The neutral particles must be identified as the bound states of the kink-antikink configurations that start and end at the same vacuum $|a\rangle$, i.e. $|K_{ab}(\theta_1)K_{ba}(\theta_2)\rangle$, with the "tooth" shapes shown in Fig. 3.

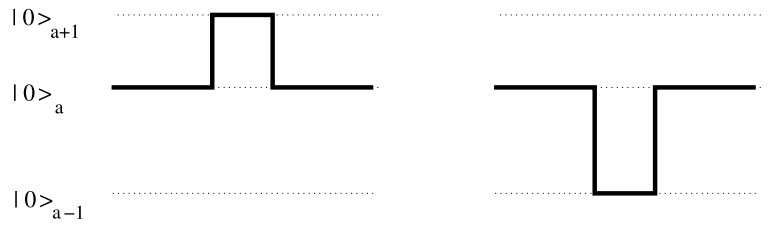

Fig. 3 Kink-antikink configurations which may give rise to a bound state nearby the vacuum $|0\rangle_a$

If such two-kink states have a pole at an imaginary value iu^c_{ab} within the physical strip $0 < \mathrm{Im}\,\theta < \pi$ of their rapidity difference $\theta = \theta_1 - \theta_2$, then their bound states are defined through the factorization formula which holds in the vicinity of this singularity

$$|K_{ab}(\theta_1)K_{ba}(\theta_2)\rangle \simeq i\frac{g^c_{ab}}{\theta - iu^c_{ab}}|B_c\rangle_a. \tag{7}$$

In this expression g^c_{ab} is the on-shell 3-particle coupling between the kinks and the neutral particle. Moreover, the mass of the bound states is simply obtained by substituting the resonance value iu^c_{ab} within the expression of the Mandelstam variable s of the two-kink channel

$$s = 4M^2_{ab}\cosh^2\frac{\theta}{2} \quad \longrightarrow \quad m_c = 2M_{ab}\cos\frac{u^c_{ab}}{2}. \tag{8}$$

Concerning the vacua themselves, as well known, in the infinite volume their classical degeneracy is removed by selecting one of them, say $|k\rangle$, out of the n available. This happens through the usual spontaneously symmetry breaking mechanism, even though—strictly speaking—there may be no internal symmetry to break at all. This is the case, for instance, of the potential shown in Fig. 1, which does not have any particular invariance. In the absence of a symmetry which connects the various vacua, the world—as seen by each of them—may appear very different: they can have, indeed, different particle contents. The problem we would like to examine in this talk concerns the neutral excitations around each vacuum, in particular the question of the existence of such particles and of the value of their masses. To this aim, let's make use of a semiclassical approach.

2 A Semiclassical Formula

The starting point of our analysis is a remarkably simple formula due to Goldstone-Jackiw [17], which is valid in the semiclassical approximation, i.e. when the coupling constant goes to zero and the mass of the kinks becomes correspondingly very large with respect to any other mass scale. In its refined version, given in [19] and rediscovered in [25], it reads as follows[1] (Fig. 4)

$$f^{\varphi}_{ab}(\theta) = \langle K_{ab}(\theta_1)|\varphi(0)|K_{ab}(\theta_2)\rangle \simeq \int_{-\infty}^{\infty} dx e^{iM_{ab}\theta x}\varphi_{ab}(x), \tag{9}$$

where $\theta = \theta_1 - \theta_2$.

[1] The matrix element of the field $\varphi(y)$ is easily obtained by using $\varphi(y) = e^{-iP_\mu y^\mu}\varphi(0)e^{iP_\mu y^\mu}$ and by acting with the conserved energy-momentum operator P_μ on the kink state. Moreover, for the semiclassical matrix element $F^{\mathcal{G}}_{ab}(\theta)$ of the operator $G[\varphi(0)]$, one should employ $G[\varphi_{ab}(x)]$. For instance, the matrix element of $\varphi^2(0)$ are given by the Fourier transform of $\varphi^2_{ab}(x)$.

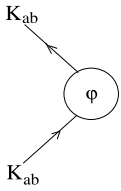

Fig. 4 Matrix element between kink states

Notice that, if we substitute in the above formula $\theta \to i\pi - \theta$, the corresponding expression may be interpreted as the following Form Factor

$$F_{ab}^{\varphi}(\theta) = f(i\pi - \theta) = \langle a|\varphi(0)|K_{ab}(\theta_1)K_{ba}(\theta_2)\rangle. \tag{10}$$

In this matrix element, it appears the neutral kink states around the vacuum $|a\rangle$ we are interested in.

Equation (9) deserves several comments.

1. The appealing aspect of the formula (9) stays in the relation between the Fourier transform of the *classical* configuration of the kink,—i.e. the solution $\varphi_{ab}(x)$ of the differential equation (2)—to the *quantum* matrix element of the field $\varphi(0)$ between the vacuum $|a\rangle$ and the 2-particle kink state $|K_{ab}(\theta_1)K_{ba}(\theta_2)\rangle$.

   Once the solution of (2) has been found and its Fourier transform has been taken, the poles of $F_{ab}(\theta)$ within the physical strip of θ identify the neutral bound states which couple to φ. The mass of the neutral particles can be extracted by using (8), while the on-shell 3-particle coupling g_{ab}^{c} can be obtained from the residue at these poles (Fig. 5)

$$\lim_{\theta \to i u_{ab}^{c}} \left(\theta - i u_{ab}^{c}\right) F_{ab}(\theta) = i g_{ab}^{c} \langle a|\varphi(0)|B_c\rangle. \tag{11}$$

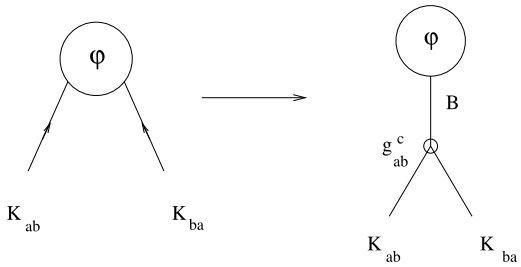

Fig. 5 Residue equation for the matrix element on the kink states

2. It is important to stress that, for a generic theory, the classical kink configuration $\varphi_{ab}(x)$ is not related in a simple way to the anti-kink configuration $\varphi_{ba}(x)$. It

is precisely for this reason that neighbouring vacua may have a different spectrum of neutral excitations, as shown in the examples discussed in the following sections.

3. It is also worth noting that this procedure for extracting the bound states masses permits in many cases to avoid the semiclassical quantization of the breather solutions [5, 6], making their derivation much simpler. The reason is that, the classical breather configurations depend also on time and have, in general, a more complicated structure than the kink ones. Yet, it can be shown that in non-integrable theories these configurations do not exist as exact solutions of the partial differential equations of the field theory. On the contrary, in order to apply (9), one simply needs the solution of the *ordinary* differential (2). It is worth notice that, to locate the poles of $f_{ab}^{\varphi}(\theta)$, one only needs to looking at the exponential behavior of the classical solutions at $x \to \pm\infty$, as discussed below.

In the next two sections we will present the analysis of a class of theories with only two vacua, which can be either symmetric or asymmetric ones. A complete analysis of other potentials can be found in the original paper [24].

3 Symmetric Wells

A prototype example of a potential with two symmetric wells is the φ^4 theory in its broken phase. The potential is given in this case by

$$U(\varphi) = \frac{\lambda}{4}\left(\varphi^2 - \frac{m^2}{\lambda}\right)^2. \tag{12}$$

Let us denote with $|\pm 1\rangle$ the vacua corresponding to the classical minima $\varphi_{\pm}^{(0)} = \pm\frac{m}{\sqrt{\lambda}}$. By expanding around them, $\varphi = \varphi_{\pm}^{(0)} + \eta$, we have

$$U\left(\varphi_{\pm}^{(0)} + \eta\right) = m^2\eta^2 \pm m\sqrt{\lambda}\eta^3 + \frac{\lambda}{4}\eta^4. \tag{13}$$

Hence, perturbation theory predicts the existence of a neutral particle for each of the two vacua, with a bare mass given by $m_b = \sqrt{2}m$, irrespectively of the value of the coupling λ. Let's see, instead, what is the result of the semiclassical analysis.

The kink solutions are given in this case by

$$\varphi_{-a,a}(x) = a\frac{m}{\sqrt{\lambda}}\tanh\left[\frac{mx}{\sqrt{2}}\right], \quad a = \pm 1 \tag{14}$$

and their classical mass is

$$M_0 = \int_{-\infty}^{\infty} \epsilon(x)dx = \frac{2\sqrt{2}}{3}\frac{m^3}{\lambda}. \tag{15}$$

The value of the potential at the origin, which gives the height of the barrier between the two vacua, can be expressed as

$$U(0) = \frac{3m}{8\sqrt{2}} M_0, \tag{16}$$

and, as noticed in the introduction, is proportional to the classical mass of the kink.

If we take into account the contribution of the small oscillations around the classical static configurations, the kink mass gets corrected as [5, 6]

$$M = \frac{2\sqrt{2}}{3}\frac{m^3}{\lambda} - m\left(\frac{3}{\pi\sqrt{2}} - \frac{1}{2\sqrt{6}}\right) + \mathcal{O}(\lambda). \tag{17}$$

It is convenient to define

$$c = \left(\frac{3}{2\pi} - \frac{1}{4\sqrt{3}}\right) > 0,$$

and also the adimensional quantities

$$g = \frac{3\lambda}{2\pi m^2}; \qquad \xi = \frac{g}{1 - \pi c g}. \tag{18}$$

In terms of them, the mass of the kink can be expressed as

$$M = \frac{\sqrt{2}m}{\pi\xi} = \frac{m_b}{\pi\xi}. \tag{19}$$

Since the kink and the anti-kink solutions are equal functions (up to a sign), their Fourier transforms have the same poles. Hence, the spectrum of the neutral particles will be the same on both vacua, in agreement with the Z_2 symmetry of the model. We have

$$f_{-a,a}(\theta) = \int_{-\infty}^{\infty} dx e^{iM\theta x} \varphi_{-a,a}(x) = ia\sqrt{\frac{2}{\lambda}} \frac{1}{\sinh(\frac{\pi M}{\sqrt{2}m}\theta)}.$$

By making now the analytical continuation $\theta \to i\pi - \theta$ and using the above definitions (18), we arrive to

$$F_{-a,a}(\theta) = \langle a|\varphi(0)|K_{-a,a}(\theta_1)K_{a,-a}(\theta_2)\rangle \propto \frac{1}{\sinh(\frac{(i\pi-\theta)}{\xi})}. \tag{21}$$

The poles of the above expression are located at

$$\theta_n = i\pi\,(1 - \xi n)\,, \quad n = 0, \pm 1, \pm 2, \ldots \tag{22}$$

and, if

$$\xi \geq 1, \tag{23}$$

none of them is in the physical strip $0 < \mathrm{Im}\,\theta < \pi$. Consequently, in the range of the coupling constant

$$\frac{\lambda}{m^2} \geq \frac{2\pi}{3}\frac{1}{1+\pi c} = 1.02338\ldots \tag{24}$$

the theory does not have any neutral bound states, neither on the vacuum to the right nor on the one to the left. Viceversa, if $\xi < 1$, there are $n = [\frac{1}{\xi}]$ neutral bound states, where $[x]$ denote the integer part of the number x. Their semiclassical masses are given by

$$m_b^{(n)} = 2M \sin\left[n\frac{\pi\xi}{2}\right] = n m_b\left[1 - \frac{3}{32}\frac{\lambda^2}{m^4}n^2 + \cdots\right]. \tag{25}$$

Note that the leading term is given by multiples of the mass of the elementary boson $|B_1\rangle$. Therefore the n-th breather may be considered as a loosely bound state of n of it, with the binding energy provided by the remaining terms of the above expansion. But, for the non-integrability of the theory, all particles with mass $m_n > 2m_1$ will eventually decay. It is easy to see that, if there are at most two particles in the spectrum, it is always valid the inequality $m_2 < 2m_1$. However, if $\xi < \frac{1}{3}$, for the higher particles one always has

$$m_k > 2m_1, \quad \text{for } k = 3, 4, \ldots, n. \tag{26}$$

According to the semiclassical analysis, the spectrum of neutral particles of φ^4 theory is then as follows: (i) if $\xi > 1$, there are no neutral particles; (ii) if $\frac{1}{2} < \xi < 1$, there is one particle; (iii) if $\frac{1}{3} < \xi < \frac{1}{2}$ there are two particles; (iv) if $\xi < \frac{1}{3}$ there are $[\frac{1}{\xi}]$ particles, although only the first two are stable, because the others are resonances.

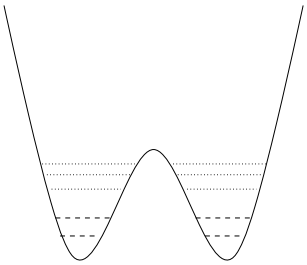

Fig. 6 Neutral bound states of φ^4 theory for $g < 1$. The lowest two lines are the stable particles whereas the higher lines are the resonances

Let us now briefly mention some general features of the semiclassical methods, starting from an equivalent way to derive the Fourier transform of the kink solution. To simplify the notation, let's get rid of all possible constants and consider the Fourier transform of the derivative of the kink solution, expressed as

$$G(k) = \int_{-\infty}^{\infty} dx e^{ikx} \frac{1}{\cosh^2 x}. \tag{27}$$

We split the integral in two terms

$$G(k) = \int_{-\infty}^{0} dx e^{ikx} \frac{1}{\cosh^2 x} + \int_{0}^{\infty} dx e^{ikx} \frac{1}{\cosh^2 x}, \tag{28}$$

and we use the following series expansion of the integrand, valid on the entire real axis (except the origin)

$$\frac{1}{\cosh^2 x} = 4 \sum_{n=1}^{\infty} (-1)^{n+1} n e^{-2n|x|}. \tag{29}$$

Substituting this expression into (28) and computing each integral, we have

$$G(k) = 4i \sum_{n=1}^{\infty} (-1)^{n+1} n \left[-\frac{1}{ik + 2n} + \frac{1}{-ik + 2n} \right]. \tag{30}$$

Obviously it coincides with the exact result, $G(k) = \pi k / \sinh \frac{\pi}{2} k$, but this derivation permits to easily interpret the physical origin of each pole. In fact, changing k to the original variable in the crossed channel, $k \to (i\pi - \theta)/\xi$, we see that the poles which determine the bound states at the vacuum $|a\rangle$ are only those relative to the exponential behaviour of the kink solution at $x \to -\infty$. This is precisely the point where the classical kink solution takes values on the vacuum $|a\rangle$. In the case of φ^4, the kink and the antikink are the same function (up to a minus sign) and therefore they have the same exponential approach at $x = -\infty$ at both vacua $|\pm 1\rangle$. Mathematically speaking, this is the reason for the coincidence of the bound state spectrum on each of them: this does not necessarily happens in other cases, as we will see in the next section, for instance.

The second comment concerns the behavior of the kink solution near the minima of the potential. In the case of φ^4, expressing the kink solution as

$$\varphi(x) = \frac{m}{\sqrt{\lambda}} \tanh \left[\frac{mx}{\sqrt{2}} \right] = \frac{m}{\sqrt{\lambda}} \frac{e^{\sqrt{2}x} - 1}{e^{\sqrt{2}x} + 1}, \tag{31}$$

and expanding around $x = -\infty$, we have

$$\varphi(t) = -\frac{m}{\sqrt{\lambda}} \left[1 - 2t + 2t^2 - 2t^3 + \cdots + 2(-1)^n t^n \cdots \right], \tag{32}$$

where $t = \exp[\sqrt{2}x]$. Hence, all the sub-leading terms are exponential factors, with exponents which are multiple of the first one. Is this a general feature of the kink solutions of any theory? It can be proved that the answer is indeed positive [24].

The fact that the approach to the minimum of the kink solutions is always through multiples of the same exponential (when the curvature ω at the minimum is different

from zero) implies that the Fourier transform of the kink solution has poles regularly spaced by $\xi_a \equiv \frac{\omega}{\pi M_{ab}}$ in the variable θ. If the first of them is within the physical strip, the semiclassical mass spectrum derived from the formula (9) near the vacuum $|a\rangle$ has therefore the universal form

$$m_n = 2M_{ab} \sin\left(n\frac{\pi\xi_a}{2}\right). \tag{33}$$

As we have previously discussed, this means that, according to the value of ξ_a, we can have only the following situations at the vacuum $|a\rangle$: (a) no bound state if $\xi_a > 1$; (b) one particle if $\frac{1}{2} < \xi_a < 1$; (c) two particles if $\frac{1}{3} < \xi_a < \frac{1}{2}$; (d) $[\frac{1}{\xi_a}]$ particles if $\xi_a < \frac{1}{3}$, although only the first two are stable, the others being resonances. So, semiclassically, each vacuum of the theory cannot have more than two stable particles above it. Viceversa, if $\omega = 0$, there are no poles in the Fourier transform of the kink and therefore there are no neutral particles near the vacuum $|a\rangle$.

4 Asymmetric Wells

In order to have a polynomial potential with two asymmetric wells, one must necessarily employ higher powers than φ^4. The simplest example of such a potential is obtained with a polynomial of maximum power φ^6, and this is the example discussed here. Apart from its simplicity, the φ^6 theory is relevant for the class of universality of the Tricritical Ising Model [30]. As we can see, the information available on this model will turn out to be a nice confirmation of the semiclassical scenario. .

A class of potentials which may present two asymmetric wells is given by

$$U(\varphi) = \frac{\lambda}{2}\left(\varphi + a\frac{m}{\sqrt{\lambda}}\right)^2\left(\varphi - b\frac{m}{\sqrt{\lambda}}\right)^2\left(\varphi^2 + c\frac{m^2}{\lambda}\right), \tag{34}$$

with a, b, c all positive numbers. To simplify the notation, it is convenient to use the dimensionless quantities obtained by rescaling the coordinate as $x^\mu \to mx^\mu$ and the field as $\varphi(x) \to \sqrt{\lambda}/m\varphi(x)$. In this way the Lagrangian of the model becomes

$$\mathscr{L} = \frac{m^6}{\lambda^2}\left[\frac{1}{2}(\partial\varphi)^2 - \frac{1}{2}(\varphi + a)^2(\varphi - b)^2(\varphi^2 + c)\right]. \tag{35}$$

The minima of this potential are localized at $\varphi_0^{(0)} = -a$ and $\varphi_1^{(0)} = b$ and the corresponding ground states will be denoted by $|0\rangle$ and $|1\rangle$. The curvature of the potential at these points is given by

$$\begin{aligned} U''(-a) \equiv \omega_0^2 &= (a+b)^2(a^2+c); \\ U''(b) \equiv \omega_1^2 &= (a+b)^2(b^2+c). \end{aligned} \tag{36}$$

For $a \neq b$, we have two asymmetric wells, as shown in Fig. 7. To be definite, let's assume that the curvature at the vacuum $|0\rangle$ is higher than the one at the vacuum $|1\rangle$, i.e. $a > b$.

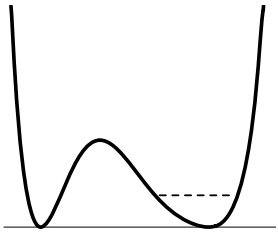

Fig. 7 Example of φ^6 potential with two asymmetric wells and a bound state only on one of them

The problem we would like to examine is whether the spectrum of the neutral particles $|B\rangle_s$ ($s = 0, 1$) may be different at the two vacua, in particular, whether it would be possible that one of them (say $|0\rangle$) has no neutral excitations, whereas the other has just one neutral particle. The ordinary perturbation theory shows that both vacua has neutral excitations, although with different value of their mass:

$$m^{(0)} = (a+b)\sqrt{2(a^2+c)}, \qquad m^{(1)} = (a+b)\sqrt{2(b^2+c)}. \tag{37}$$

Let's see, instead, what is the semiclassical scenario. The kink equation is given in this case by

$$\frac{d\varphi}{dx} = \pm(\varphi + a)(\varphi - b)\sqrt{\varphi^2 + c}. \tag{38}$$

We will not attempt to solve exactly this equation but we can present nevertheless its main features. The kink solution interpolates between the values $-a$ (at $x = -\infty$) and b (at $x = +\infty$). The anti-kink solution does vice versa, but with an important difference: its behaviour at $x = -\infty$ is different from the one of the kink. As a matter of fact, the behaviour at $x = -\infty$ of the kink is always equal to the behaviour at $x = +\infty$ of the anti-kink (and vice versa), but the two vacua are approached, in this theory, differently. This is explicitly shown in Fig. 8 and proved in the following.

Let us consider the limit $x \to -\infty$ of the kink solution. For these large values of x, we can approximate (38) by substituting, in the second and in the third term of the right-hand side, $\varphi \simeq -a$, with the result

$$\left(\frac{d\varphi}{dx}\right)_{0,1} \simeq (\varphi + a)(a+b)\sqrt{a^2+c}, \quad x \to -\infty. \tag{39}$$

This gives rise to the following exponential approach to the vacuum $|0\rangle$

$$\varphi_{0,1}(x) \simeq -a + A\exp(\omega_0 x), \quad x \to -\infty \tag{40}$$

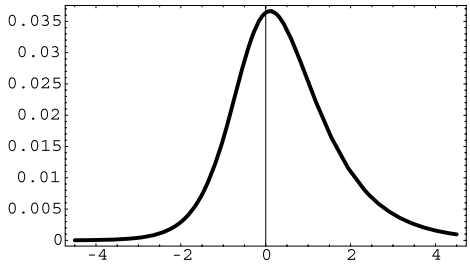

Fig. 8 Typical shape of $(\frac{d\varphi}{dx})_{01}$, obtained by a numerical solution of (38)

where $A > 0$ is a arbitrary constant (its actual value can be fixed by properly solving the non-linear differential equation). To extract the behavior at $x \to -\infty$ of the anti-kink, we substitute this time $\varphi \simeq b$ into the first and third term of the right hand side of (38), so that

$$\left(\frac{d\varphi}{dx}\right)_{1,0} \simeq (\varphi - b)(a + b)\sqrt{b^2 + c}, \quad x \to -\infty. \tag{41}$$

This ends up in the following exponential approach to the vacuum $|1\rangle$

$$\varphi_{1,0}(x) \simeq b - B\exp(\omega_1 x), \quad x \to -\infty \tag{42}$$

where $B > 0$ is another constant. Since $\omega_0 \neq \omega_1$, the asymptotic behaviour of the two solutions gives rise to the following poles in their Fourier transform

$$\begin{aligned} \mathscr{F}(\varphi_{0,1}) &\to \frac{A}{\omega_0 + ik}, \\ \mathscr{F}(\varphi_{1,0}) &\to \frac{-B}{\omega_1 + ik}. \end{aligned} \tag{43}$$

In order to locate the pole in θ, we shall reintroduce the correct units. Assuming to have solved the differential equation (38), the integral of its energy density gives the common mass of the kink and the anti-kink. In terms of the constants in front of the Lagrangian (35), its value is given by

$$M = \frac{m^5}{\lambda^2}\alpha, \tag{44}$$

where α is a number (typically of order 1), coming from the integral of the adimensional energy density (4). Hence, the first pole[2] of the Fourier transform of the kink and the antikink solution are localized at

[2] In order to determine the others, one should look for the subleading exponential terms of the solutions.

$$\begin{aligned}\theta^{(0)} &\simeq i\pi\left(1-\omega_0\frac{m}{\pi M}\right)=i\pi\left(1-\omega_0\frac{\lambda^2}{\alpha m^4}\right),\\ \theta^{(1)} &\simeq i\pi\left(1-\omega_1\frac{m}{\pi M}\right)=i\pi\left(1-\omega_1\frac{\lambda^2}{\alpha m^4}\right).\end{aligned} \tag{45}$$

If we now choose the coupling constant in the range

$$\frac{1}{\omega_0}<\frac{\lambda^2}{m^4}<\frac{1}{\omega_1}, \tag{46}$$

the first pole will be out of the physical sheet whereas the second will still remain inside it! Hence, the theory will have only one neutral bound state, localized at the vacuum $|1\rangle$. This result may be expressed by saying that the appearance of a bound state depends on the order in which the topological excitations are arranged: an antikink-kink configuration gives rise to a bound state whereas a kink-antikink does not.

Finally, notice that the value of the adimensional coupling constant can be chosen so that the mass of the bound state around the vacuum $|1\rangle$ becomes equal to mass of the kink. This happens when

$$\frac{\lambda^2}{m^4}=\frac{\alpha}{3\omega_1}. \tag{47}$$

Strange as it may appear, the semiclassical scenario is well confirmed by an explicit example. This is provided by the exact scattering theory of the Tricritical Ising Model perturbed by its sub-leading magnetization. Firstly discovered through a numerical analysis of the spectrum of this model [21], its exact scattering theory has been discussed later in [2].

5 Conclusions

In this paper we have used simple arguments of the semi-classical analysis to investigate the spectrum of neutral particles in quantum field theories with kink excitations. We have concentrated our analysis on two cases: the first relative to a potential with symmetric wells, the second concerning with a potential with asymmetric wells. Leaving apart the exact values of the quantities extracted by the semiclassical methods, it is perhaps more important to underline some general features which have emerged through this analysis. One of them concerns, for instance, the existence of a critical value of the coupling constant, beyond which there are no neutral bound states. Another result is about the maximum number $n \leq 2$ of neutral particles living on a generic vacuum of a non-integrable theory. An additional aspect is the role played by the asymmetric vacua, which may have a different number of neutral excitations above them.

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Exponential Decay Laws in Perturbation Theory of Threshold and Embedded Eigenvalues

Arne Jensen and Gheorghe Nenciu

Abstract Exponential decay laws for the metastable states resulting from perturbation of unstable eigenvalues are discussed. Eigenvalues embedded in the continuum as well as threshold eigenvalues are considered. Stationary methods are used, i.e. the evolution group is written in terms of the resolvent via Stone's formula and a partition technique (Schur-Livsic-Feschbach-Grushin formula) is used to localize the essential terms. No analytic continuation of the resolvent is required. The main result is about the threshold case: for Schrödinger operators in odd dimensions the leading term of the life-time in the perturbation strength, ε, is of order $\varepsilon^{2+\nu/2}$, where ν is an odd integer, $\nu \geq -1$. Examples covering all values of ν are given. For eigenvalues properly embedded in the continuum the results sharpen the previous ones.

1 Introduction

Let H be a self-adjoint operator in a Hilbert space $\mathcal{H}$ and E_0 a finitely degenerate eigenvalue of H: $HP_0 = E_0P_0$, $\dim P_0 < \infty$. On $P_0\mathcal{H}$ the evolution is stationary:

$$P_0e^{-itH}P_0 = e^{-itE_0}P_0. \tag{1}$$

The problem we consider is what happens with the evolution compressed to $P_0\mathcal{H}$, when a perturbation is added, i.e. H is replaced by

$$H_\varepsilon = H + \varepsilon W. \tag{2}$$

Arne Jensen
Department of Mathematical Sciences, Aalborg University, Fr. Bajers Vej 7G, 9220 Aalborg O, Denmark, e-mail: matarne@math.aau.dk

Gheorghe Nenciu
Faculty of Physics, University of Bucharest, P.O. Box MG 11, 077125 Bucharest, Romania and Institute of Mathematics of the Romanian Academy, P.O. Box 1-764, 014700 Bucharest, Romania, e-mail: Georghe.Nenciu@imar.ro

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On heuristic grounds one expects that

$$P_0 e^{-itH_\varepsilon} P_0 = e^{-ith_\varepsilon} P_0 + \delta(\varepsilon, t), \tag{3}$$

where h_ε is a (dissipative) "effective hamiltonian" in $P_0\mathcal{H}$ and $\delta(\varepsilon, t)$ is an error term vanishing in the limit $\varepsilon \to 0$.

Among the questions to be answered are:

(i) Find sufficient conditions for (3) to hold true. In particular one can ask whether there are interesting cases, in which such a simple description of the compressed dynamics does not exist (e.g. non exponential decay laws).
(ii) Compute the effective Hamiltonian h_ε.
(iii) Estimate

$$\sup_{t>0} \|\delta(\varepsilon, t)\| = \delta(\varepsilon). \tag{4}$$

The above questions can be completely answered in the elementary case of a regular perturbation of discrete eigenvalues. Here the Kato-Rellich analytic perturbation theory gives

$$h_\varepsilon = h_\varepsilon^* = U_\varepsilon^* P_\varepsilon H_\varepsilon P_\varepsilon U_\varepsilon, \tag{5}$$

$$\delta(\varepsilon) \leq \text{const} \cdot \varepsilon^2, \tag{6}$$

where P_ε is the perturbed projection, and U_ε is the Sz.-Nagy transformation matrix of the pair P_ε, P_0 (see e.g. [18]). Moreover, one can show that (6) is optimal, i.e. the power of ε in the error term cannot exceed 2. One remark is in order here. One can ask whether h_ε as given by (3) and (4) is unique. The answer is no, and one can easily see that if one takes $\tilde{h}_\varepsilon = W_\varepsilon^* h_\varepsilon W_\varepsilon$ with W_ε unitary, $[W_\varepsilon, P_0] = 0$, and $\|W_\varepsilon - 1\| \leq \text{const} \cdot \varepsilon^2$, then $\tilde{h}_\varepsilon$ still satisfies (3) and (6). However, there is a uniqueness statement: the spectrum, $\sigma(h_\varepsilon)$, must coincide with the spectrum of H_ε emerging from E_0, i.e. h_ε is unique up to a unitary rotation.

Consider now the really interesting case, when E_0 is embedded (properly or at a threshold) in the continuous spectrum of H or/and W is singular with respect to H, as e.g. in the Stark effect. A fairly complete answer is known in the case of dilation analytic Hamiltonians, if in addition one supposes that E_0 is not situated at a threshold. More precisely, using the analytic perturbation theory in the framework of Aguilar-Balslev-Combes dilation analytic Hamiltonians, as developed by Simon [25], Hunziker [9] proved that (3) with the estimate (6) holds true. The important point here is that h_ε is no more self-adjoint, but only dissipative, which reflects the fact that generically under the effect of the perturbation the stationary state becomes metastable with (up to a uniform error of order ε^2) an exponential decay law. In the non-degenerate case (3) gives the rigorous foundation (control on error term included!) for the famous survival probability formula (here $h_\varepsilon = \lambda_\varepsilon P_0$)

$$|\langle \Psi_0, e^{-itH_\varepsilon} \Psi_0 \rangle|^2 \sim e^{-2|\operatorname{Im} \lambda_\varepsilon| t}, \tag{7}$$

as given by the Dirac second order time dependent perturbation theory (Fermi Golden Rule).

The question we address is to what extent Hunziker's results can be generalized to:

(i) A non-analytic (smooth) context.
(ii) Threshold eigenvalues.

Our main interest is in the threshold eigenvalues case (however we shall give also results for properly embedded eigenvalues, extending and sharpening the existing ones). While for properly embedded eigenvalues one has a (generically) universal behavior as $\varepsilon \to 0$ of the decay rate constant, $\Gamma_\varepsilon \equiv 2|\operatorname{Im}\lambda_\varepsilon| \sim \varepsilon^2$, given by the "universal" Fermi Golden Rule, for threshold eigenvalues the situation is by far more complicated. As remarked by Baumgartner [2], even at the heuristic level the usual Fermi Golden Rule prescription to compute the decay rate constant does not work. The deep reason is that in the neighborhood of a threshold the resolvent (Green's function) has a complicated non universal structure. After all it is well known that quantum mechanics at threshold is a tricky business! It turns out that contrary to the properly embedded eigenvalue case, for threshold eigenvalues the behavior as $\varepsilon \to 0$ of Γ_ε is (generically) not universal; in the Schrödinger operators case it depends upon the dimension of the space, angular momentum, as well as upon the existence of threshold resonances.

Our main result [14] is that for threshold eigenvalues of Schrödinger operators in odd dimensions, the leading term of the decay rate constant in the perturbation strength, ε, is of order $\varepsilon^{2+\nu/2}$, where ν is an odd integer, $\nu \geq -1$. We give examples for all values of ν, for which we compute the leading term in Γ_ε, and give estimates for the error term.

There are basically two general approaches to derive (3). The first one, initiated by Soffer and Weinstein [26], consists in a direct study of the Schrödinger evolution governed by H_ε:

$$i\,\partial_t \psi(t) = H_\varepsilon \psi(t) \tag{8}$$

for initial conditions localized in energy around E_0. The second one, initiated by Orth [24], is the stationary approach, which by use of the Stone formula reduces the computation of the l.h.s. of (3) to the computation of an integral over energies involving the compressed resolvent. In both methods, in order to isolate the significant contributions, one uses variants of projection techniques (appearing in the literature under various names as: Liapunov-Schmidt projection method, Schur complements, Livsic-Feschbach matrix, Grushin method, etc; for more comments and references see [14]).

We use the stationary approach. We refine it as to cover the threshold eigenvalues case (and also to sharpen the existing results for properly embedded eigenvalues) by adding two things:

(i) Detailed asymptotic expansions near a threshold of the resolvent of Schrödinger operators in odd dimensions obtained in [10, 11, 22, 14, 12, 13].
(ii) A careful study of the integral appearing in the Stone formula, especially regarding the interval of energies giving the significant contributions.

Finally we would like to stress that we do not touch here the huge field related to resonances, from the spectral-scattering theory point of view. For further references we send the reader to [8, 23], as well as to the recent review [7].

2 The Basic Formula

The first step is to localize in energy. Thus we consider $P_0 e^{-itH_\varepsilon} g_\varepsilon(H_\varepsilon) P_0$, where $0 \leq g_\varepsilon(x) \leq 1$ is the (possibly smoothed) characteristic function of an interval in a neighborhood of E_0. The crucial point here is the following beautiful, elementary remark due to Hunziker [9]:

Proposition 1. *Suppose that for some* $h_\varepsilon : P_0\mathcal{H} \to P_0\mathcal{H}$,

$$\| P_0 e^{-itH_\varepsilon} g_\varepsilon(H_\varepsilon) P_0 - e^{-ith_\varepsilon} P_0 \| \leq \delta(\varepsilon). \tag{9}$$

Then

$$\| P_0 e^{-itH_\varepsilon} P_0 - e^{-ith_\varepsilon} P_0 \| \leq 2\delta(\varepsilon). \tag{10}$$

Then one can use the freedom of choice of $g_\varepsilon(x)$ to be able to compute h_ε, and to optimize the error estimate. We note that usually $g_\varepsilon(x)$ is chosen independent of ε. One of the key points of our approach is to make an appropriate *ε-dependent* choice of $g_\varepsilon(x)$. For example, in the case of perturbing threshold eigenvalues, it is crucial that $g_\varepsilon(x)$ is the characteristic function of an interval, which is "far" from the threshold, i.e. does not contain the unperturbed eigenvalue. In what follows we choose an interval $I_\varepsilon = (e_0(\varepsilon) - d(\varepsilon), e_0(\varepsilon) + d(\varepsilon))$, and take $g_\varepsilon(x) = \chi_{I_\varepsilon}(x)$ as the cut-off function. As already said the central point in our approach is to find the "right" location $e_0(\varepsilon)$, and the "right" size function $d(\varepsilon)$, such that energies in I_ε give the resonance behavior, and energies outside I_ε only contribute to the error term $\delta(\varepsilon, t)$.

A remark is in order here. By taking a smoothed out characteristic function one can obtain a refinement of (10) in the form

$$P_0 e^{-itH_\varepsilon} P_0 = (I + A(\varepsilon)) e^{-ith_\varepsilon} (I + A(\varepsilon)) + \delta(\varepsilon, t),$$

where $A(\varepsilon) = \mathcal{O}(\varepsilon^p)$ for some $p > 0$, and $\delta(\varepsilon, t)$ now exhibits decay in t for t large. However, our concern here is with error estimates uniform in time, so we take just the characteristic function as our cut-off function.

The next step is to write down a workable formula for the compressed evolution in (9). For this purpose we use the Stone formula to express the compressed evolution in terms of compressed resolvent, and then we use the Schur-Livsic-Feschbach-Grushin (SLFG) partition formula to express the compressed resolvent as an inverse. We briefly recall the SLFG formula (for details, further references, and historical remarks, we send the reader to [14]). Let $R_\varepsilon(z) = (H(\varepsilon) - z)^{-1}$, and let $R_{0,\varepsilon}(z)$ be the resolvent of $Q_0 H(\varepsilon) Q_0$, as an operator in $Q_0\mathcal{H}$, where

$$Q_0 = 1 - P_0. \tag{11}$$

Then we have in the decomposed space $\mathcal{H} = P_0\mathcal{H} \oplus Q_0\mathcal{H}$

$$R_\varepsilon(z) = \begin{bmatrix} R_{\text{eff}}(z) & -\varepsilon R_{\text{eff}}(z) P_0 W Q_0 R_{0,\varepsilon}(z) \\ -\varepsilon R_{0,\varepsilon}(z) Q_0 W P_0 R_{\text{eff}}(z) & R_{22} \end{bmatrix}, \tag{12}$$

with

$$R_{\text{eff}}(z) = \left(P_0 H(\varepsilon) P_0 - \varepsilon^2 P_0 W Q_0 R_{0,\varepsilon}(z) Q_0 W P_0 - z P_0\right)^{-1}.$$

We do not give the formula for R_{22}, since it is not needed here, see [14] for this formula.

More precisely, by using the Stone formula, the SLFG formula, and by rearranging the Neumann series for the perturbed resolvent, one arrives at the following basic formula for the compressed evolution [14]:

Proposition 2.

$$\begin{aligned} P_0 e^{-itH_\varepsilon} g_\varepsilon(H_\varepsilon) P_0 &= \lim_{\eta\to 0} \frac{1}{\pi} \int dx e^{-itx} g_\varepsilon(x) \operatorname{Im} P_0 (H_\varepsilon - x - i\eta)^{-1} P_0 \\ &= \lim_{\eta\to 0} \frac{1}{\pi} \int dx\, e^{-itx} g_\varepsilon(x) \operatorname{Im} F(x + i\eta, \varepsilon)^{-1} \end{aligned} \tag{13}$$

where using the notation

$$W = A^* D A, \quad D = D^* = D^{-1}, \tag{14}$$

$$G(z) = A Q_0 (H - z)^{-1} Q_0 A^*, \tag{15}$$

as an operator in $P_0\mathcal{H}$, the function $F(z, \varepsilon)$ is given by

$$\begin{aligned} F(z, \varepsilon) = (E_0 - z) P_0 + \varepsilon P_0 W P_0 - \varepsilon^2 P_0 A^* D G(z) D A P_0 \\ + \varepsilon^3 P_0 A^* D G(z) [D + \varepsilon G(z)]^{-1} G(z) D A P_0. \end{aligned} \tag{16}$$

The formulas (13) and (16) are the starting formulas of our approach, and at this point the hard work starts. What is needed is to show that on the interval I_ε, up to a controllable error, $F(x + i\eta, \varepsilon) = h_\varepsilon - x - i\eta$, so that one can isolate the resonant term and estimate the remainder. All that depends crucially on the smoothness properties of $F(z, \varepsilon)$. The main point of the formula (16) is that $F(z, \varepsilon)$ inherits the smoothness properties of $G(z)$. This allows, assuming appropriate conditions on $G(z)$, to prove "semi-abstract" results, and then apply them to various concrete cases, by checking these assumptions. In what follows the assumptions for the threshold case are modeled on Schrödinger operators in odd dimensions.

3 The Results

3.1 Properly Embedded Eigenvalues

Let for $a > 0$

$$D_a(E_0) = \{z \in \mathbf{C} | |z - E_0| < a, \operatorname{Im} z > 0\}. \tag{17}$$

We denote by $C^{n,\theta}(D_a(E_0))$ the functions in $D_a(E_0)$ that are n times continuously norm-differentiable, with the n^{th} derivative satisfying a uniform Hölder condition in $D_a(E_0)$, of order θ, $0 \leq \theta \leq 1$. The main assumption in this subsection is that

$$G(z) \in C^{n,\theta}(D_a(E_0)). \tag{18}$$

Such conditions can be verified in an abstract setting, using the Mourre estimate and the multiple commutator technique, see e.g. [1, 3, 6], and references therein. Note this assumption implies that $G(z)$ has boundary values $G(x + i0)$, which are in $C^{n,\theta}((E_0 - a, E_0 + a))$. For Schrödinger operators the smoothness of $G(z)$ also follows, if the potential decays sufficiently fast at infinity.

We give first the result in the non-degenerate case [14].

Theorem 1. *Assume $G(z) \in C^{n,\theta}(D_a(E_0))$. Assume $\dim P_0 = 1$ and $n + \theta > 0$. Write $F(x+i0, \varepsilon) = (R(x, \varepsilon)+i I(x, \varepsilon))P_0$. Then for ε sufficiently small there exists a (unique for $n + \theta \geq 1$) solution to $R(x, \varepsilon) = 0$ in the interval $(E_0 - a, E_0 + a)$, denoted by $x_0(\varepsilon)$. Let $\Gamma(\varepsilon) = I(x_0(\varepsilon), \varepsilon)$, write*

$$\lambda_\varepsilon = x_0(\varepsilon) - i\Gamma(\varepsilon), \tag{19}$$

and let Ψ_0 denote a normalized eigenfunction for eigenvalue E_0 of H. Then for ε sufficiently small, and for all $t > 0$, the following results hold true:

(i) *Assume $n = 0$, $0 < \theta < 1$, and*

$$\Gamma(\varepsilon) \geq C\varepsilon^\gamma \quad \text{with } 2 \leq \gamma < \frac{2}{1-\theta}. \tag{20}$$

Then we have

$$|\langle \Psi_0, e^{-itH(\varepsilon)}\Psi_0\rangle - e^{-it(x_0(\varepsilon)-i\Gamma(\varepsilon))}| \leq C\frac{1}{1-\theta}\varepsilon^\delta, \tag{21}$$

where

$$\delta = 2 - \gamma(1-\theta) > 0. \tag{22}$$

(ii) *For $n + \theta \geq 1$ we have*

$$|\langle \Psi_0, e^{-itH(\varepsilon)}\Psi_0\rangle - e^{-it(x_0(\varepsilon)-i\Gamma(\varepsilon))}| \leq C \begin{cases} \varepsilon^2|\ln\varepsilon| & \text{for } n = 0, \theta = 1, \\ \varepsilon^2 & \text{for } n + \theta > 1. \end{cases} \tag{23}$$

The results in the theorem above sharpen and amplify similar results in [5, 4, 19–21, 26, 27]. Let us stress that in the high regularity case, i.e. $n + \theta \geq 1$, there is no lower bound condition for $\Gamma(\varepsilon)$. In particular, λ_ε can be an eigenvalue.

We turn now to the degenerate case. In the degenerate case the results are by far less complete. In particular, in order to prove (3) and (4), one has to impose a condition on the size of the imaginary part of $\mathrm{Im}\, F(E_0 + i0)$, namely the so-called Fermi Golden Rule condition (see (24) below). One can relax (24), if one imposes conditions on the spectrum of $P_0 W P_0$, such that one can apply the methods and results from the non-degenerate case [24, 16]. Our main result [16] here sharpening the ones in [21, 28] is contained in

Theorem 2. *Assume $N \geq 2$ and $G(z) \in C^{n,\theta}(D_a(E_0))$ with $n + \theta \geq 2$. Assume there exists $\gamma > 0$ such that*

$$\mathrm{Im}\, P_0 A^* DG(E_0 + i0) DA P_0 \geq \gamma P_0. \tag{24}$$

Then there exists a function $\delta(\varepsilon, t)$ satisfying (4) with $p = 2$, such that

$$P_0 e^{-itH_\varepsilon} P_0 = e^{-ith_\varepsilon} P_0 + \delta(\varepsilon, t). \tag{25}$$

Here h_ε on $P_0\mathcal{H}$ is given by

$$\begin{aligned} h_\varepsilon = {} & E_0 P_0 + \varepsilon P_0 W P_0 - \varepsilon^2 P_0 W Q_0 (H - E_0 - i0)^{-1} Q_0 W P_0 \\ & - \varepsilon^3 \Big\{ P_0 W Q_0 (H - E_0 - i0)^{-1} Q_0 W Q_0 (H - E_0 - i0)^{-1} Q_0 W P_0 \\ & + \frac{1}{2} \Big[P_0 W P_0 W \frac{d}{dE} Q_0 (H - E - i0)^{-1} Q_0 \Big|_{E=E_0} W P_0 \\ & + P_0 W \frac{d}{dE} Q_0 (H - E - i0)^{-1} Q_0 \Big|_{E=E_0} W P_0 W P_0 \Big] \Big\}. \end{aligned} \tag{26}$$

3.2 Threshold Eigenvalues

As already said in the Introduction, the usual methods to prove the smoothness of $G(z)$ do not work at thresholds, and actually it may not be smooth, or even blows up, in the neighborhood of the origin. The way out from this difficulty is to use the asymptotic expansion of $G(z)$ around the threshold (see [10–13, 22] and references therein). Let us stress that the asymptotic expansions of the resolvent around thresholds are not universal; e.g. in the Schrödinger case the type of expansions depend on dimension, and on the threshold spectral properties of the Hamiltonian. The asymptotic expansion in the assumption below (see [14, Sect. 3]) is modeled after Schrödinger and Dirac operators in odd dimensions.

Assumption 1.

(A1) *There exists $a > 0$, such that $(-a, 0) \subset \rho(H)$ (the resolvent set) and $[0, a] \subset \sigma_{\rm ess}(H)$.*

(A2) *Assume that zero is a non-degenerate eigenvalue of H: $H\Psi_0 = 0$, with $\|\Psi_0\| = 1$, and there are no other eigenvalues in $[0, a]$. Let $P_0 = |\Psi_0\rangle\langle\Psi_0|$ be the orthogonal projection onto the one-dimensional eigenspace.*

(A3) *Assume*

$$\langle \Psi_0, W\Psi_0\rangle = b > 0. \tag{27}$$

(A4) *For $\operatorname{Re}\kappa \geq 0$ and $z \in \mathbf{C} \setminus [0, \infty)$ we let*

$$\kappa = -i\sqrt{z}, \quad z = -\kappa^2. \tag{28}$$

There exist $N \in \mathbf{N}$ and $\delta_0 > 0$, such that for $\kappa \in \{\kappa \in \mathbf{C} \,|\, 0 < |\kappa| < \delta_0, \operatorname{Re}\kappa \geq 0\}$ we have

$$G(z) = \sum_{j=-1}^{N} \widetilde{G}_j \kappa^j + \kappa^{N+1} \widetilde{G}_N(\kappa), \tag{29}$$

where

$$\widetilde{G}_j \quad \text{are bounded and self-adjoint}, \tag{30}$$

$$\widetilde{G}_{-1} \quad \text{is of finite rank and self-adjoint}, \tag{31}$$

$$\widetilde{G}_N(\kappa) \quad \text{is uniformly bounded in } \kappa. \tag{32}$$

From (29) we get

$$\langle \Psi_0, A^* DG(z) DA\Psi_0\rangle = \sum_{j=-1}^{N} g_j \kappa^j + \kappa^{N+1} g_N(\kappa), \tag{33}$$

where

$$g_j = \langle \Psi_0, A^* D\widetilde{G}_j DA\Psi_0\rangle, \tag{34}$$

$$g_N(\kappa) = \langle \Psi_0, A^* D\widetilde{G}_N(\kappa) DA\Psi_0\rangle. \tag{35}$$

(A5) *There exists an odd integer, $-1 \leq \nu \leq N$, such that*

$$g_\nu \neq 0, \quad \widetilde{G}_j = 0 \quad \text{for } j = -1, 1, \ldots, \nu - 2. \tag{36}$$

The main (semi)-abstract result dealing with threshold case is as follows [14]:

Theorem 3. *Let $x_0(\varepsilon)$, $\Gamma(\varepsilon)$ be as in Theorem 1. Suppose* (A1)–(A5) *in Assumption 1 hold true. Then for sufficiently small $\varepsilon > 0$ we have*

$$|\langle \Psi_0, e^{-itH_\varepsilon}\Psi_0\rangle - e^{-it(x_0(\varepsilon) - i\Gamma(\varepsilon))}| \leq C\varepsilon^{p(\nu)}. \tag{37}$$

Here $p(\nu) = \min\{2, (2+\nu)/2\}$, *and*

$$\Gamma(\varepsilon) = -i^{\nu-1} g_\nu b^{\nu/2} \varepsilon^{2+\nu/2}(1 + \mathcal{O}(\varepsilon)), \tag{38}$$

$$x_0(\varepsilon) = b\varepsilon(1 + \mathcal{O}(\varepsilon)). \tag{39}$$

4 A Uniqueness Result

The spectrum of the effective Hamiltonian, h_ε, (λ_ε in the nondegenerate case) gives information about the "location" of resonances resulting from the perturbation of stationary states, as can be seen in the cases, when one can define the resonances as poles of the analytic continuation of the resolvent or the scattering matrix. Then a natural question is to ask, to what extent the effective Hamiltonian h_ε as *defined* by (3) and (4) is unique. If h_ε has an asymptotic expansion as $\varepsilon \to 0$, the question is how many expansion coefficients are uniquely determined. The following result [3, 17] gives the answer to this problem.

Theorem 4.

I. *Assume* Rank $P_0 = 1$.

Assume that h_ε^1 *and* h_ε^2 *both satisfy* (3) *and* (4), *with the same value for* p. *Assume that for some* $c_0 > 0$ *and* $q > 0$ *we have*

$$-c_0 \varepsilon^q P_0 \le \operatorname{Im} h_\varepsilon^1 \le 0 \quad \text{for } 0 \le \varepsilon < \varepsilon_0. \tag{40}$$

Then for ε_0 *sufficiently small we have*

$$\|h_\varepsilon^1 - h_\varepsilon^2\|_{\mathcal{B}(P_0\mathcal{H})} \le C\varepsilon^{p+q}, \quad 0 \le \varepsilon < \varepsilon_0. \tag{41}$$

II. *Assume* $1 \le \text{Rank } P_0 < \infty$.

(i) *Assume that* h_ε^1 *and* h_ε^2 *both satisfy* (3) *and* (4), *with the same value for* p. *Assume that* h_ε^1 *satisfies*

$$h_\varepsilon^1 = E_0 P_0 + \varepsilon h_1^1 + \varepsilon f^1(\varepsilon), \quad 0 \le \varepsilon < \varepsilon_0, \tag{42}$$

such that $h_1^1 = (h_1^1)^*$, $\operatorname{Im} f^1(\varepsilon) \le 0$, *and* $f^1(\varepsilon) = o(1)$ *as* $\varepsilon \to 0$. *Assume that* h_ε^2 *is a bounded family of operators on* $P_0\mathcal{H}$. *Then for* ε_0 *sufficiently small we have*

$$\|h_\varepsilon^1 - h_\varepsilon^2\|_{\mathcal{B}(P_0\mathcal{H})} \le C\varepsilon^{p+1}, \quad 0 \le \varepsilon < \varepsilon_0. \tag{43}$$

(ii) *Assume that* h_ε^1 *and* h_ε^2 *both satisfy* (3) *and* (4), *with* $p = 2$. *Assume that* h_ε^1 *satisfies*

$$h_\varepsilon^1 = E_0 P_0 + \varepsilon h_1 + \varepsilon^2 h_2 + o(\varepsilon^2), \quad 0 \le \varepsilon < \varepsilon_0, \tag{44}$$

such that $h_1 = h_1^*$ *and* $\operatorname{Im} h_\varepsilon^1 \le 0$. *Assume that* h_ε^2 *is a bounded family of operators on* $P_0\mathcal{H}$. *Then there exists a family of invertible operators* $U(\varepsilon)$ *on* $P_0\mathcal{H}$ *with* $U(\varepsilon) = P_0 + O(\varepsilon^2)$, *such that for* ε_0 *sufficiently small we have*

$$\|h_\varepsilon^1 - U(\varepsilon)^{-1} h_\varepsilon^2 U(\varepsilon)\|_{\mathcal{B}(P_0\mathcal{H})} \leq C\varepsilon^4, \quad 0 \leq \varepsilon < \varepsilon_0. \tag{45}$$

5 Examples

In this section, for all $\nu = -1, 1, 3, \ldots$, we give examples for which Assumption 1 holds true, and then Theorem 3 gives (3) with $|\operatorname{Im}\lambda_\varepsilon| \sim \varepsilon^{2+\frac{\nu}{2}}$. In each case we compute the leading term g_ν. As examples we consider one and two channel Schrödinger operators in three dimensions [14]. For more examples, see [14–16].

5.1 Example 1: One Channel Case, $\nu = -1$

In this case

$$H = -\Delta + V(\mathbf{x}), \tag{46}$$

$$(Wf)(\mathbf{x}) = W(\mathbf{x}) f(\mathbf{x}), \tag{47}$$

in $L^2(\mathbf{R}^3)$, with V, W satisfying

$$\langle\cdot\rangle^\beta V \in L^\infty(\mathbf{R}^m), \tag{48}$$

$$\langle\cdot\rangle^\gamma W \in L^\infty(\mathbf{R}^m), \tag{49}$$

and β, γ are sufficiently large (see below). Here $E_0 = 0$. About H we suppose that it has a non-degenerate threshold eigenvalue

$$(-\Delta + V)\Psi_0 = 0, \quad \|\Psi_0\| = 1, \tag{50}$$

as well as a threshold resonance with canonical resonance function Ψ_c. We recall that H has a threshold resonance if there exist additional non-zero solutions to $(-\Delta + V)\Psi = 0$, in the space $L^{2,-s}(\mathbf{R}^3)$, $1/2 < s \leq 3/2$. Among these solutions, one can choose a distinguished one, Ψ_c, called the *canonical zero resonance function*, and all the others can be written as $\Psi = \alpha\Psi_c + \tilde{\Psi}$ with $\alpha \neq 0$ and $\tilde{\Psi} \in L^2(\mathbf{R}^3)$ (for definition and further details see [14, Appendix A]). In the theorem below we take Ψ_0 to be real-valued.

Theorem 5. *Assume that V and W satisfy* (48) *and* (49) *with $\beta > 9$ and $\gamma > 5$, respectively. Assume that* (A1–3) *holds for $H = -\Delta + V$. Let*

$$X_j = \int_{\mathbf{R}^3} \Psi_0(\mathbf{x}) V(\mathbf{x}) x_j d\mathbf{x}, \quad j = 1, 2, 3. \tag{51}$$

Assume either that $X_j \neq 0$ for at least one j, or that $\langle\Psi_0, W\Psi_c\rangle \neq 0$. Then $\nu = -1$, and we have

$$g_{-1} = \frac{b^2}{12\pi}(X_1^2 + X_2^2 + X_3^2) + |\langle \Psi_0, W\Psi_c\rangle|^2. \tag{52}$$

If H does not have a resonance at the threshold, but still $X_j \neq 0$ for at least one j, then the second term in the right hand side of (52) should be omitted, i.e.

$$g_{-1} = \frac{b^2}{12\pi}(X_1^2 + X_2^2 + X_3^2). \tag{53}$$

The following example shows the significance of the conditions in the theorem. Take

$$V(\mathbf{x}) = \begin{cases} -V_0, & \text{if } |\mathbf{x}| \leq 1, \\ 0, & \text{if } |\mathbf{x}| > 1. \end{cases}$$

Here $V_0 > 0$ is a parameter. By adjusting this parameter, one can get a radial solution to $(-\Delta + V)\psi = 0$ for any angular momentum $\ell = 0, 1, \ldots$, which decays as $|\mathbf{x}|^{-\ell}$, as $|\mathbf{x}| \to \infty$. Thus for $\ell = 0$ we get a zero resonance. For $\ell = 1$ we get zero eigenvalues, such that at least one $X_j \neq 0$, see (51). For $\ell \geq 2$ all $X_j = 0$. For $\ell \geq 1$ the eigenvalue at zero is not simple. Examples with a simple zero eigenvalue can be obtained using only the radial part. Note that in order to get $\langle \Psi_0, W\Psi_c\rangle \neq 0$ one will have to take a non-radial perturbation W.

5.2 Example 2: Two Channel Case, $v = -1, 1$

In the two channel case we consider examples of a non-degenerate bound state of zero energy in the "closed" channel decaying due to the interaction with a three dimensional Schrödinger operator in the open channel. Since only the bound state in the closed channel is relevant in the forthcoming discussion, we shall take $\mathbf{C}$ as the Hilbert space representing the closed channel, i.e. $\mathcal{H} = L^2(\mathbf{R}^3) \oplus \mathbf{C}$. As the unperturbed Hamiltonian we take

$$H = \begin{bmatrix} -\Delta + V & 0 \\ 0 & 0 \end{bmatrix}, \tag{54}$$

where V satisfies (48), and as the perturbation we take

$$W = \begin{bmatrix} W_{11} & |W_{12}\rangle\langle 1| \\ |1\rangle\langle W_{12}| & b \end{bmatrix}, \tag{55}$$

which is a shorthand for

$$W \begin{bmatrix} f(\mathbf{x}) \\ \xi \end{bmatrix} = \begin{bmatrix} W_{11}(\mathbf{x}) f(\mathbf{x}) + W_{12}(\mathbf{x})\xi \\ \int \overline{W_{12}(\mathbf{x})} f(\mathbf{x}) + b\xi \end{bmatrix}. \tag{56}$$

Here we assume

$$\langle\cdot\rangle^{\gamma} W_{11} \in L^{\infty}(\mathbf{R}^m), \quad \langle\cdot\rangle^{\gamma/2} W_{12} \in L^{\infty}(\mathbf{R}^m), \tag{57}$$

and furthermore that W_{11} is real-valued. In order to satisfy (27) we assume $b > 0$ in (55).

Concerning the two channel case we have the following result.

Theorem 6. *Assume that V and W satisfy (48) and (49) with $\beta > 9$ and $\gamma > 5$, respectively.*

(i) *Assume that $-\Delta + V$ has neither a threshold resonance nor a threshold eigenvalue. Then $\nu \geq 1$, and we have*

$$g_1 = \frac{-1}{4\pi} |\langle W_{12}, (I + G_0^0 V)^{-1} 1\rangle|^2. \tag{58}$$

where the integral kernel of G_0^0 is $\frac{1}{4\pi|\mathbf{x}-\mathbf{y}|}$.

(ii) *Assume that $-\Delta + V$ has a threshold resonance, and no threshold eigenvalue. Let Ψ_c denote the canonical zero resonance function. Assume that $\langle W_{12}, \Psi_c\rangle \neq 0$. Then $\nu = -1$, and*

$$g_{-1} = |\langle W_{12}, \Psi_c\rangle|^2. \tag{59}$$

5.3 Example 3: Two Channel Radial Case, $\nu \geq 3$

Here we consider radial part of Schrödinger operator with spherical symmetric potentials for angular momentum $\ell = 1, 2, \ldots$

$$H_{0,\ell} = -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2}, \quad \ell = 1, 2, \ldots, \tag{60}$$

on the space $\mathcal{H} = L^2(\mathbf{R}_+)$ in the two channel set-up, where we now take the Hilbert space $\mathcal{H} = L^2(\mathbf{R}_+) \oplus \mathbf{C}$, and replace (54) by

$$H = \begin{bmatrix} H_{0,\ell} & 0 \\ 0 & 0 \end{bmatrix}. \tag{61}$$

It will provide us with examples of resolvent expansions, where we can verify Assumption (A5) with $\nu \geq 3$ odd and arbitrarily large. Note that the cases $\nu = -1$ and $\nu = 1$ were covered in the preceding examples.

Theorem 7. *Consider the two channel case with H given by (61). Assume that W given by (55) satisfies (57) with $\gamma > 2\ell + 5$. Assume that*

$$\langle W_{12}, r^{\ell+1}\rangle \neq 0.$$

Then we have $\nu = 2\ell + 1$ and

$$g_v = (-1)^{\ell+1} \left[\frac{\sqrt{\pi}}{2^{\ell+1}\Gamma(\ell + \frac{3}{2})} \right]^2 |\langle W_{12}, r^{\ell+1} \rangle|^2, \tag{62}$$

where Γ denotes the usual Gamma function.

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Energy Diffusion and Superdiffusion in Oscillators Lattice Networks

Stefano Olla

Abstract I review some recent results on the thermal conductivity of chains of oscillators whose Hamiltonian dynamics is perturbed by a noise conserving energy and momentum.

1 Introduction

Let us consider a 1-dimensional chain of oscillators indexed by $x \in \mathbb{Z}$, whose formal Hamiltonian is given by

$$\mathcal{H}(p,q) = \sum_x \left[\frac{p_x^2}{2} + V(q_{x+1} - q_x) + W(q_x) \right], \tag{1}$$

where q_x indicate the displacement of the atom x from its equilibrium position, and p_x its momentum (we fix for the moment all masses equal to 1). The potential V and W are some smooth positive function growing at infinity fast enough. The W potential is often called *pinning*.

We want to understand the *macroscopic* properties of energy transport for the corresponding Hamiltonian dynamics

$$\dot{q}_x = p_x, \qquad \dot{p}_x = -\partial_{q_x}\mathcal{H}. \tag{2}$$

When we say "macroscopic energy transport" we are meaning a certain non-equilibrium evolution that we want to observe in a space-time macroscopic scale that should be specified. This space-time scale can be typical of the model and the same model can have distinct macroscopic scalings under which it will behave very dif-

Stefano Olla
Ceremade, UMR CNRS 7534, Université de Paris Dauphine, Place du Maréchal De Lattre De Tassigny, 75775 Paris Cedex 16, France, e-mail: olla@ceremade.dauphine.fr

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ferently. For example in the case that $W = 0$ (unpinned system), total momentum is also conserved and hyperbolic scaling (in which space and time are scaled in the same way) is a natural one. In the hyperbolic scaling, energy is carried around by the momentum of the particles and macroscopic evolution equation is given by the Euler equations.

Another important scaling is the diffusive scaling (time scaled as square of space) where transport of energy happens by diffusion. The macroscopic equation is usually given by heat equation. For example, when the pinning potential W is present, total momentum is not conserved and nothing moves in the hyperbolic scale. Energy will *move* on the diffusive space-time scale, and macroscopically its evolution should be governed by heat equation. More precisely, defining the empirical distribution of the energy

$$\tilde{\mathcal{E}}^{\varepsilon}(G,t) = \varepsilon \sum_x G(\varepsilon x)\mathcal{E}_x(\varepsilon^{-2}t) \tag{3}$$

where $\mathcal{E}_x = \frac{p_x^2}{2} + V(q_{x+1} - q_x) + W(q_x)$ is the energy of particle x, and G is a smooth test function on $\mathbb{R}$ with compact support. We expect that

$$\lim_{\varepsilon \to 0} \tilde{\mathcal{E}}^{\varepsilon}(G,t) = \int G(y)u(y,t)\,dy \tag{4}$$

in *some statistical sense*, with $u(y,t)$ solution of the (non-linear) heat equation

$$\partial_t u = \partial_x(\kappa(u)\partial_x u). \tag{5}$$

The function $\kappa(u)$ is called thermal conductivity and can be expressed in terms of the dynamics in equilibrium:

$$\kappa(u) = \lim_{t\to\infty} \frac{1}{2tT^2} \sum_x x^2[\langle \mathcal{E}_x(t)\mathcal{E}(0)\rangle_T - u^2] \tag{6}$$

where the temperature $T = T(u)$ correspond thermodynamically to the average energy u, $< \cdot >_T$ is the expectation of the dynamics in equilibrium at temperature T.

Proving (4)–(5) from an Hamiltonian microscopic dynamics is one of the major challenge in non-equilibrium statistical mechanics [8]. It is not clear under which conditions on the interaction and initial conditions this result could be valid. Even the proof of the existence of the limit (6) defining the thermal conductivity is completely open for any deterministic system. What is clear is that (4)–(5) are not always valid. For example if V and W are quadratic (harmonic chains), then the energy corresponding to each Fourier mode is conserved and carried ballistically without any interaction with the other modes. It results that thermal conductivity is infinite in this case ([16], and for a macroscopic equation in the hyperbolic scaling see [9], as explained in Sect. 4).

In nonlinear unpinned cases ($W = 0$) one expects, generically in dimension 1, that $\kappa = +\infty$, and correspondingly a superdiffusion of energy. This fact seems con-

firmed by all numerical simulation of molecular dynamics [12], even though there is not a general agreement about the order of this superdiffusivity. Most interesting would be to understand what kind of stochastic process would govern this superdiffusion.

Adding a stochastic perturbation to the Hamiltonian dynamics certainly helps to obtain some mathematical result in these problems. Of course adding noise to the microscopic dynamics may change the macroscopic behavior. The ideal is to add noise terms that change as little as possible the macroscopic behaviour, at least qualitatively. For example it is important that this noise conserves energy, and eventually momentum, since these are the quantities we expect being *conserved* by the infinite system.

2 Conservative Stochastic Dynamics

We consider the Hamiltonian dynamics weakly perturbed by a stochastic noise acting only on momenta and locally preserving momentum and kinetic energy. The generator of the dynamics is

$$L = A + \gamma S \tag{7}$$

with $\gamma > 0$, where A is the usual Hamiltonian vector field

$$A = \sum_{yx \in \mathbb{Z}} \{p_x \partial_{q_x} - (\partial_{q_x} \mathcal{H}) \partial_{p_x}\}, \tag{8}$$

while S is the generator of the stochastic perturbation. The operator S acts only on the momenta $\{p_y\}$ and generates a diffusion on the surface of constant kinetic energy and constant momentum. S is defined as

$$S = \frac{1}{6} \sum_{z \in \mathbb{Z}} (Y_z)^2, \tag{9}$$

where

$$Y_z = (p_z - p_{z+1}) \partial_{p_{z-1}} + (p_{z+1} - p_{z-1}) \partial_{p_z} + (p_{z-1} - p_z) \partial_{p_{z+1}}$$

which is a vector field tangent to the surface of constant kinetic energy and of constant momentum for three neighbouring particles. As a consequence energy and momentum are locally conserved which, of course, implies also the conservation of total momentum and total energy of the system, i.e. formally

$$S \sum_{x \in \mathbb{Z}} p_x = 0, \qquad S\mathcal{H} = 0.$$

Since also the Hamiltonian dynamics conserves energy, we also have $L\mathcal{H} = 0$. Furthermore in the unpinned case ($W = 0$), $L \sum_x p_x = 0$.

The evolution of $\{p(t), q(t)\}$ is given by the following stochastic differential equations

$$\begin{aligned} dq_x &= p_x dt, \\ dp_x &= -\partial_x \mathcal{H} dt + \frac{\gamma}{6} \Delta(4p_x + p_{x-1} + p_{x+1}) dt \\ &\quad + \sqrt{\frac{\gamma}{3}} \sum_{k=-1,0,1} (Y_{x+k} p_x) dw_{x+k}(t). \end{aligned} \tag{10}$$

Here $\{w_y(t)\}_{y\in\mathbb{Z}}$ are independent standard Wiener processes and Δ is the discrete Laplacian on $\mathbb{Z}$: $\Delta f(z) = f(z+1) + f(z-1) - 2f(z)$.

In the unpinned 1-dimensional case, the equilibrium measures are particularly simple. In fact the right coordinates are $r_x = q_{x+1} - q_x$, and the family of product measures

$$\mu_{\lambda,p,\beta}(dp, dr) = \prod_{x\in\mathbb{Z}} \frac{e^{-\beta(p_x - p)^2/2}}{\sqrt{2\pi}} \frac{e^{-\beta V(r_x) + \lambda r_x}}{Z(\lambda, \beta)} \tag{11}$$

are stationary for the dynamics. The three parameters λ, p, β correspond to the 3 conserved quantities of the dynamics (energy, momentum and $\sum_x r_x$, the *stretch* of the chain), while $Z(\lambda, \beta)$ is the normalization constant. It can be proven that these are the only translation invariant stationary measures of the dynamics ([6], we call this property "ergodicity of the infinite dynamics"). In more dimensions the unpinned case is much more complex and even the definition of these equilibrium measures are problematic (cf. [10]).

In the unpinned one-dimensional case, since momentum is conserved, there is a non trivial macroscopic evolution on the conserved quantities in the hyperbolic scaling (space and time scaled in the same way). Let us define the energy of particle x as

$$\mathcal{E}_x = \frac{p_x^2}{2} + \frac{1}{2}(V(r_{x-1}) + V(r_x)).$$

Locally the conservation of energy can be written as

$$L\mathcal{E}_x = j^{\mathcal{E}}_{x-1,x} - j^{\mathcal{E}}_{x,x+1} \tag{12}$$

where the instantaneous current of energy $j^{\mathcal{E}}_{x,x+1}$ is the sum of the current due to the Hamiltonian mechanism plus the current due to the stochastic term of the dynamics:

$$\begin{aligned} j^{\mathcal{E}}_{x,x+1} &= j^{\mathcal{E},a}_{x,x+1} + j^{\mathcal{E},s}_{x,x+1} \\ j^{\mathcal{E},a}_{x,x+1} &= -\frac{1}{2}(p_x + p_{x+1}) V'(r_x), \qquad j^{\mathcal{E},s}_{x,x+1} = -\gamma \nabla \varphi_x \end{aligned} \tag{13}$$

with $\varphi_x = (p_{x+1}^2 + 4p_x^2 + p_{x-1}^2 + p_{x+1}p_{x-1} - 2p_{x+1}p_x - 2p_x p_{x-1})$. Similarly conservation of momentum reads as

$$\begin{aligned} Lp_x &= j^p_{x-1,x} - j^p_{x,x+1}, \\ j^p_{x,x+1} &= V'(r_x) + \frac{\gamma}{6}\nabla(4p_x + p_{x-1} + p_x) \end{aligned} \tag{14}$$

while mass conservation is simply given by

$$Lr_x = p_{x+1} - p_x. \tag{15}$$

Let $G(y)$ a test function continuous with compact support. We expect that

$$\epsilon \sum_x G(\epsilon x) \begin{pmatrix} r_x(\epsilon^{-1}t) \\ p_x(\epsilon^{-1}t) \\ \mathcal{E}_x(\epsilon^{-1}t) \end{pmatrix} \overset{\text{probability}}{\underset{\epsilon\to 0}{\longrightarrow}} \int G(y) \begin{pmatrix} \mathfrak{r}(t,y) \\ \mathfrak{p}(t,y) \\ \mathfrak{e}(t,y) \end{pmatrix} dy \tag{16}$$

where $\mathfrak{r}(t,y), \mathfrak{p}(t,y), \mathfrak{e}(t,y)$ are given by the solution of the Euler hyperbolic system of equations

$$\begin{aligned} \partial_t \mathfrak{r} &= \partial_y \mathfrak{p} \\ \partial_t \mathfrak{p} &= \partial_y P(\mathfrak{r}, \mathfrak{e} - \mathfrak{p}^2/2) \\ \partial_t \mathfrak{e} &= \partial_y \Big(\mathfrak{p} P(\mathfrak{r}, \mathfrak{e} - \mathfrak{p}^2/2) \Big). \end{aligned} \tag{17}$$

Here $P(r,u)$ is the thermodynamic pressure, which is related to the thermodynamic entropy $S(r,u)$ by the relation

$$P(r,u) = -\frac{\partial_r S(r,u)}{\partial_u S(r,u)} \tag{18}$$

and S is defined from $Z(\lambda,\beta)$ with a Legendre transform:

$$S(r,u) = \sup_{\lambda,\beta} \big\{ \lambda r - \beta u - \log\big(Z(\lambda,\beta)\sqrt{\beta/2\pi} \big) \big\}. \tag{19}$$

Pressure $P(r,u)$ is also given by the expectation of $V'(r_x)$ with respect to $\mu_{\lambda,p,\beta}$, for the corresponding values of the parameters λ and β.

The hydrodynamic limit (16) can be proven rigorously in the smooth regime of equation (17), by using the relative entropy method ([14], see also [1] and [6] for the application to this specific model). Note that (16) does not depend on the strength of the microscopic noise γ. Noise here is used only to prove some ergodic properties for the dynamics, necessary to obtain the result. In fact without noise this limit may not be true, as for example in the linear case (V quadratic, see below). Note also that for smooth solutions the macroscopic evolution (17) is locally isoentropic, i.e.

$$\frac{d}{dt} S\left(\mathfrak{r}(t,y), \mathfrak{e}(t,y) - \frac{\mathfrak{p}(t,y)^2}{2} \right) = 0. \tag{20}$$

A challenging open problem is to extend this result to solutions that present shocks, where the above derivative is (presumably) strictly positive.

3 Diffusive Evolution: Green-Kubo Formula

In the pinned model ($W > 0$) momentum is not conserved, energy is the only relevant conserved quantity for the infinite system and the equilibrium measure are the Gibbs measures at given temperature, corresponding to the Hamiltonian $\mathcal{H}$. These probability measures are defined by the usual DLR equations. Consequently the hyperbolic scaling is trivial (nothing moves at that time scale). In order to see energy moving at a macroscopic scale, one has to look at larger time scale. The natural scaling is the diffusive one: we expect, for a given test function G as above,

$$\epsilon \sum_x G(\epsilon x)\mathcal{E}_x(\epsilon^{-2}t) \overset{\text{probability}}{\underset{\epsilon\to 0}{\longrightarrow}} \int G(y)\mathfrak{T}(t,y)\,dy \tag{21}$$

where $\mathfrak{T}(t,y)$ is the solution of the (non-linear) heat equation

$$\partial_t \mathfrak{T} = \partial_x(\kappa(\mathfrak{T})\partial_x\mathfrak{T}) \tag{22}$$

where $\kappa(T)$ is the thermal conductivity at temperature T. This is given by the Green-Kubo formula

$$\kappa(T) = \frac{1}{2\chi(T)}\left[\int_0^\infty \sum_{x=-\infty}^{+\infty} \left\langle j^{\mathcal{E},a}_{x,x+1}(t)\, j^{\mathcal{E},a}_{0,1}(0)\right\rangle_T dt + \gamma T^2\right] \tag{23}$$

where $\langle j^{\mathcal{E},a}_{x,x+1}(t)\, j^{\mathcal{E},a}_{0,1}(0)\rangle_T$ denote the expectation with respect to the dynamics in equilibrium at temperature $T = \beta^{-1}$. The explicit $\gamma T^2/2\chi(T)$ term is the contribution of the stochastic part of the dynamics. Formula (23) can be obtained from (6) using the conservation of energy (see [3] for a proof). We believe that such statement is always true for non-linear pinned dynamics, also in the deterministic case ($\gamma = 0$). But even for $\gamma > 0$, this is hard to prove and still an open problem. Even the convergence of the integrals defining (23) is not known if non-linearities are present (some bounds are proven in [3]). The only case with non-linear interaction in which (23) is proven convergent is when the noise is generated by Langevin heat bath attached at each particle of the system [7], a non conservative stochastic perturbation.

In unpinned systems the situation is more complex because of the momentum conservation. To avoid complicate re-centering along characteristics of (17), we can consider initial random configurations with momentum of (locally) zero average and constant density profile, only gradients of temperature admitted. Then conductivity κ is also a function of the density of particles and in formula (23) the expectation should be taken with respect to the equilibrium dynamics with $p = 0$ (i.e. starting with configurations distributed by $\mu_{\lambda,0,\beta}$ defined by (11)). Numerical evidence shows that in this one-dimensional case $\kappa = +\infty$ ([12], also for $\gamma > 0$, as long as momentum is conserved [4]). In the physics literature there is a long discussion about the nature and the *order* or this superdiffusion. From dimension 3 on, it is expected that formulas corresponding to (23) give a finite diffusivity.

Rigorous results can be proven for the harmonic case with $\gamma > 0$ [2, 3]. It turns out that κ is finite if system is pinned or in dimension $d \geq 3$, while the 1 and 2 dimensional unpinned cases are superdiffusive.

4 Kinetic Limits: Phonon Boltzmann Equation

The harmonic case is enough simple to obtain some non-equilibrium results. In [5] we consider the hyperbolic scaling in a weak noise limit. Noise is rescaled by multiplying its strength γ by ϵ. This way the effect of the noise per particle remains finite in the macroscopic scale (that motivates the term *kinetic* in defining this limit). This is in the same spirit as the model of hard sphere with random collision considered in [15]. The right quantity to look here is the Wigner distribution of the energy, formally defined as

$$W^\epsilon(y,k,t) = \frac{1}{2}\int_{-1/2}^{1/2} e^{i2\pi y\eta/\epsilon}\langle \psi(k-\eta/2, t/\epsilon)^* \psi(k+\eta/2, t/\epsilon)\rangle d\eta \qquad (24)$$

where

$$\psi(k,t) = \frac{1}{\sqrt{2}}(\omega(k)\hat{q}(k,t) + i\,\hat{p}(k,t))$$

here $\hat{q}(k,t)$, $\hat{p}(k,t)$ are the Fourier transform of the $q_y(t)$, $p_y(t)$, and $\omega(k)$ is the dispersion relation of the lattice, which in this one-dimensional nearest neighbour case is given by $\omega(k) = c|\sin(\pi k)|$ (*acoustic dispersion*). The result in [5] states that $W^\epsilon(y,k,t)$ converges, as a distribution on $\mathbb{R}\times[0,1]$, to the solution of the linear transport equation

$$\partial_t W(y,k,t) + \frac{\omega'(k)}{2\pi}\partial_y W(y,k,t) = \gamma\int C(k,k')(W(y,k',t) - W(y,k,t))dk. \qquad (25)$$

In the deterministic case ($\gamma = 0$) this result was obtained by Dobrushin et al. in [9], see also [13]. The collision kernel $C(k,k')$ is positive and symmetric. It is computable explicitly (cf. [5]), but the important point is that $C(k,k') \sim k^2$ for small k. This is a consequence of the conservation of momentum: long waves scatter very rarely. Because $C(k,k')$ is positive, (25) has a simple probabilistic interpretation: W is the density at time t of the energy of particles (phonons) of mode k. A phonon of mode k moves with velocity $\omega'(k)$ and after an exponentially distributed random time of intensity $\gamma C(k,k')$ changes its mode to k'. Defining a Markov jump process $K(t)$ in $[0,1]$ with jumping rate γC, the position of the phonons is given by $Y(t) = \int_0^t \omega'(K(s))ds$.

Thermal conductivity can be computed from (25) (cf. [5]) and the results are in accord with the direct calculations done in [3].

5 Levy's Superdiffusion of Energy

As we mention in the previous section, phonons of small k scatter rarely, but their velocity $\omega'(k)$, in the unpinned case, are still of order 1 as $k \to 0$. This induces a superdiffusive behavior of these phonons. In [11], as application of new limit theorems for functionals of Markov chains and processes, we prove that, for $\alpha = 3/2$,

$$\epsilon Y(\epsilon^{-\alpha} t) \underset{\text{law}}{\longrightarrow} \mathcal{L}(t) \tag{26}$$

where $\mathcal{L}(t)$ is a Levy α-stable process, i.e. a stochastic process with independent stationary increments and with $\mathcal{L}(1)$ distributed by a α-stable law. In terms of the solution $W(y, k, t)$ of (25) this result implies the convergence

$$\lim_{\epsilon \to 0} \int |W(\epsilon^{-\alpha} t, \epsilon^{-1} y, k) - \bar{u}(t, y)|^2 dk = 0 \tag{27}$$

where $\bar{u}(t, y)$ is the solution of the fractional heat equation

$$\partial_t \bar{u} = -c(-\Delta_y)^{\alpha/2} \bar{u}. \tag{28}$$

where c is a positive constant.

In the pinned case all the above results are still valid, but since the velocity of the phonons $\omega'(k) \sim k$ for small k, we have a regular diffusive behavior, and $\alpha = 2$.

It would be very interesting to understand how these results extends to the anharmonic cases. Equation (25) will be substituted by the non-linear phonon Boltzmann equation [17]. In the unpinned one-dimensional case this equation still will produce a superdiffusion. Is it again of Levy type, or will have some non-Markovian terms?

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Trying to Characterize Robust and Generic Dynamics

Enrique R. Pujals

Abstract If we consider that the mathematical formulation of natural phenomena always involves simplifications of the physical laws, real significance of a model may be accorded only to those properties that are robust under perturbations. In loose terms, robustness means that some main features of a dynamical system are shared by all nearby systems. In this short article, we will explain the structure related to the presence of robust transitivity and the universal mechanisms that lead to lack of robustness. Providing a conceptual framework, the goal is to show how this approach helps to describe 'generic' dynamics in the space of all dynamical systems.

1 Introduction

In a broad sense, the goal of dynamics is to describe the long term evolution of systems for which an "infinitesimal" evolution rule is known. It is natural to try to solve the "equations" by looking for analytic expressions for the trajectories, and indeed that was the prevailing point of view in differential equations until little more than a century ago. However, that turns out to be impossible in most cases, both theoretically and in practice. Moreover, even when such an analytic expressions can be found, it is usually difficult to deduce from them useful conclusions about the global dynamics. Then, by the end of the 19th century, Poincare proposed to find qualitative information on the dynamics without actually finding the solutions. Its goal will be the understanding of the essential nature of what the properties that generic mathematical equations has, rather than focusing with the equations themselves.

Enrique R. Pujals
IMPA, Estr. Dona Castorina 110, CEP 22460-320, Rio de Janeiro, R.J., Brazil, e-mail: enrique@impa.br

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Following this approach, for a long time it has been a goal in the theory of dynamical systems to describe the dynamics from the generic viewpoint, that is, describing the dynamics of "big sets" (residual, dense, etc.) of the space of all dynamical systems. In other words: *can we describe the behavior in the long run of typical trajectories for the 'majority' of systems?*

In this sense, to study a dynamic system is to look for mathematically describable patterns that a system tends to settle. These sets are sets which are "dynamically indecomposable", "invariant", and "isolated" (also called *elementary pieces*) that contain the recurrent part of the dynamic (the so called *nonwandering set*). *Invariant*, means that any trajectory starting in the set remains in the set; *dynamically indecomposable* means that the set is *transitive* (i.e., contains trajectories which are dense in the set); *isolated*, means that the set is maximal invariant (i.e., the set is given by the trajectories that for the past and the future remains in a neighborhood of the set).

During the early times of nonconservative dynamics was a common sense that "non pathological" systems behaves in a very simple form: the nonwandering set consisting of *finitely many periodic elements*. The achievement of Peixoto that an open and dense subset of C^1 vector fields on surfaces consist of the now-called Morse-Smale systems is paradigmatic of this view. However, in the early sixties (by Anosov and Smale and following Birkhoff, Cartwright and Littlewood, etc.) it was shown that "chaotic behavior" may exist within stable systems and this was the starting point of the *hyperbolic theory* and the modern nonconservative dynamical systems theory. A major result in this theory is the fact that for these systems (nowadays called *hyperbolics*, see Sect. 2.1), the nonwandering set can be decomposed into finitely many compact, disjoint and transitive pieces. Although this pieces could exhibit a chaotic behavior there are just finitely many of them and this recover the old vision by replacing finitely many periodic elements by these finitely many "non-trivial elementary" pieces.

It was soon realized that hyperbolic systems were not as universal as was initially thought: there were given examples of open sets of diffeomorphism were none of them are hyperbolic. Nevertheless in all these new examples the nonwandering set *still decompose into finitely many compact, disjoint and transitive pieces*. Moreover, this phenomena holds in a *robust* way: *Any perturbation of the initial system still has a only a finite number of transitive pieces.*

It was through the seminal work of Newhouse (see [41–43]) where a new phenomena was shown: *the existence of infinitely many periodic attractors (today called Newhouse's phenomena) for residual subsets in the space of C^r diffeomorphisms ($r \geqslant 2$) of compact surfaces*. The underlying *mechanism* here was the presence of a homoclinic bifurcation named *homoclinic tangency*: non-transversal intersection of the stable and unstable manifold of a periodic point (see Sect. 3).

In the light of those results, the following dichotomy was formulated for generic dynamics (see [1] for more details):

1. *Robust/Tame dynamics*: those having in a robust way, finitely many elementary dynamical pieces in the ambient manifold;

2. *Wild dynamics* (*Newhouse's phenomena*): those with infinitely many elementary pieces having independent dynamical behaviors.

Once the dichotomy is presented, one tried to understand the structure related to the presence of robust phenomena and the universal mechanisms that lead to lack of robustness and to wild dynamics. Following this approach, the theory moves in the ongoing directions:

1. Characterization of the properties and structure that robust (tame) dynamics have; in particular, the study and characterization of isolated transitive sets that remain transitive for all nearby systems (*robust transitivity*).
2. Characterization of the properties and structure that wild dynamics exhibit.
3. Characterization of universal mechanisms (understood as homoclinic bifurcations) that lead to robust and wild dynamics.

These problems are all related to each other and in many cases provide a conceptual framework that makes possible to understand a twofold problem: *the relation between mechanisms and phenomenas*. As we are going to show, a global panorama, although partial and very incomplete, is beginning to appear. In this approach, local mechanism are used to characterize global properties of the dynamics. In this sense, the strategy consists in building new mechanisms, enough for characterizing all the possible behaviors. Therefore, one focus is to understand which are the mechanisms that make a transitive either to be robust or to "explode/implode" in infinitely many other sets.

In the present note we focus our attention on diffeomorphism acting on a smooth boundaryless compact manifold. Some references to the flow case are also made. Moreover, the present note focus on nonconservative systems; however, we mention some results for the conservative case (recall that in this case, a long and successful theory had been developed where the KAM theorem is the major highlight).

In Sect. 2 we extend ourselves explaining the relevant examples of robust dynamics. In the three following subsections we details the main structure that those systems exhibit. In Sect. 3 we focus in the main mechanisms that generate wild dynamics and in Sect. 4 we expose partial results in the direction to describe generic type of dynamics.

2 Robust Transitivity: Hyperbolicity, Partial Hyperbolicity and Dominated Splitting

A diffeomorphisms $f : M \to M$ is robustly transitive if every diffeomorphism in a C^1 neighborhood has dense orbits. More generally:

> An invariant compact set Λ is robustly transitive if there is an open neighborhood U of Λ and a neighborhood $\mathscr{V}$ of the diffeomorphism f in $\mathrm{Diff}^1(M)$ such that for every $g \in \mathscr{V}$ the maximal invariant set $\Lambda_g = \bigcap_{n\in\mathbb{Z}} g^n(U)$ of g in U is a transitive set.

The description of these systems is an important challenge: on the one hand, being robust, they can not be ignored in any global picture of dynamical systems; on the other hand, their dynamics is often chaotic.

The typical models showing robust properties are the well known Anosov maps (as examples of global hyperbolic dynamics) and the Smale's horseshoes (as examples of local hyperbolic ones).

However, it was shown that there are open sets in the space of dynamics which are nonhyperbolic although transitive. Indeed, in [52], an open set of non-hyperbolic transitive diffeomorphisms in the 4-torus were exhibited (open sets of diffeomorphisms exhibiting hyperbolic periodic points of different indices inside a transitive set). On one hand, these examples were a serious blow at the time, since they meant that even such seemingly simple situations, exhibiting a unique dynamical piece, cannot be understood within the framework of hyperbolicity. On the other hands these systems exhibit a weaker form of hyperbolicity called *partial hyperbolicity:* the tangent bundle is allowed to split into Df-invariant subbundles $TM = E^s \oplus E^c \oplus E^u$, such that the behavior of vectors in E^s, E^u is similar to the hyperbolic case, but vectors in E^c may be neutral for the action of the tangent map. See Sect. 2.2 for more details.

But the story about robust transitivity does no finish with the partially hyperbolic ones: In the late 90's, examples of robust transitive dynamics without any hyperbolic subbundles were exhibited. More precisely, in [15] was shown that *there are robustly transitive diffeomorphisms in the* 4*-torus which have no expanding or contracting invariant sub-bundle; therefore, they are neither hyperbolic nor partially hyperbolic*. However, those examples still exhibit a some kind of structure of their tangent dynamics: there is a splitting $TM = E^{cs} \oplus E^{cu}$ preserved by the derivative of the map, called *dominated splitting*, where E^{cs} and E^{cu} are indecomposable and nonhyperbolic. See Sect. 2.3 for more details.

All those examples pushes the theory in the following directions:

1. The general characterization of isolated transitive sets that remain transitive for all nearby systems;
2. The dynamical consequences of weaker forms of hyperbolicity;
3. The characterization of universal mechanisms that could lead to robustly nonhyperbolic behavior.

Respect to the first question proposed a general principle is concluded: *robust dynamical phenomena reflect some robust structure of the tangent map*.

In fact, in [35] for surface diffeomorphisms, in [25] for dimension three, and in [17] for any dimension it is shown that this is the main characteristic of C^1-robust transitivity. More precisely, the following was proved:

> *Any C^1-robust transitive diffeomorphism exhibits a dominated splitting such that its extremal bundles are uniformly volume contracted or expanded.*

This last theorem has other formulations in terms of certain generic dichotomy and also in conservative terms: see [1, 10, 11, 13, 12, 5].

A similar theory can be developed for flows that include that includes the Geometric models for the Lorenz equations proposed in [2, 29]. Diverse results that

characterize robustly transitive flows with an equilibrium point have been developed. We refer to [38, 8, 4, 49] for further reading.

In the next subsection, we are going to extend ourselves in explaining the notion of hyperbolicity, partially hyperbolicity and dominated splitting. We also going to explain certain relevance that those models has in some physical problems: in the hyperbolic case we describe a mechanical model with hyperbolic dynamics; in the partial hyperbolic case, we explain certain construction in the context of symplectic dynamics which are relevant to the problem of Arnold's diffusion; in the context of dominated splitting, we relate these dynamics with Gaussian thermostats and isokinetic dynamics.

2.1 Hyperbolicity

The study of hyperbolicity goes back to the work of Hadamard in 1898 concerning geodesic flows for surfaces with negative curvature, showing the density of closed geodesics and the instability of the flow with respect to initial conditions. In the 20s and 30s, Hedlund and Hopf showed that these flows are topologically mixing and that they are ergodic with respect to the Liouville measure.

Later, in [3] it was shown that geodesic flows for compact manifolds with negative sectional curvature are hyperbolic (Anosov) flows.

Let us start defining the notion of hyperbolicity for diffeomorphisms: Given a compact invariant set $\Lambda \subset M$ of a diffeomorphism f, one says that *Λ is a hyperbolic set of f if the tangent bundle of Λ splits into two invariant sub-bundles: $T_\Lambda M = E^s \oplus E^u$, and there are two constants $\lambda < 0$ and $c > 0$ such that the following properties hold:*

1. $\|Df^n|_{E^s}\| < c\exp(\lambda n)$ *for $n > 0$; that is, E^s is uniformly contracted in the future.*
2. $\|Df^{-n}|_{E^u}\| < c\exp(\lambda n)$ *for $t > 0$; that is, E^u is uniformly contracted in the past.*

The classical example of hyperbolic diffeomorphisms are the Anosov ones where Λ is the whole manifold, and the Axiom A where in this case Λ is the nonwandering set and the periodic points are dense.

For a vector field X, *a compact set Λ invariant by the flow is a hyperbolic set of Φ_t if the tangent bundle of Λ splits into three invariant sub-bundles: $T_\Lambda M = E^s \oplus [X] \oplus E^u$, such that $[X]$ is the subbundle induced by the vector field, and the subbundle E^s is uniformly contracted in the future and E^u is uniformly contracted in the past.* One of the most important property of hyperbolic systems is that in contrast to the instability of their orbits, the hyperbolic dynamics are stable in the sense that any perturbation of the system is conjugate to the initial one, meaning that the relevant dynamical behavior is actually the same, in some appropriate sense, again for all nearby systems. In particular, this shows that transitive hyperbolic systems (hyperbolic systems that have a dense trajectory) are in fact C^r robust transitive ones; i.e: *any C^r small perturbation of the initial system remains transitive*.

A long standing question has been whether there is a physical example of a Hamiltonian system with Anosov energy levels—i.e., the Hamiltonian flow is Anosov on some energy level sets. A positive answer to this question was given in the remarkable paper of [31] where the dynamics of a triple linkage is studied: three disks in a plane, free to rotate about pivots fixed in a triangle, but constrained by three rods connecting one point of each disk to a pivot x. For its free frictionless motion Hunt and Mackay proved existence of an open set of three linkage configurations for which the dynamics in each positive energy level set is a geodesic Anosov flow arising from negative curvature.

2.2 Partial Hyperbolicity

Given a closed invariant set Λ we say that it is strong partially hyperbolic if $T_\Lambda M = E^{ss} \oplus E^c \oplus E^{uu}$ and there are constants $0 < \sigma^{-1} < \gamma^{-1} < 1 < \gamma < \sigma$ such that

$$\|Df_{|E^{ss}_x}\| < \sigma^{-1} < \sigma < \|Df^{-1}_{|E^{uu}}\|^{-1} \quad \forall x \in \Lambda$$
$$\|Df_{|E^{ss}_x}\| \left\| Df^{-1}_{|E^c_{f^{-1}(x)}} \right\| < \gamma^{-1}, \qquad \|Df_{|E^c_x}\| \left\| Df^{-1}_{|E^{uu}_{f^{-1}(x)}} \right\| < \gamma^{-1} \quad \forall x \in \Lambda.$$

We say that Λ is partially hyperbolic if $T_\Lambda M = E^s \oplus E^{cu}$, constants $0 < \sigma < \gamma < 1$ such that

$$\|Df_{|E^s_x}\| < \sigma, \qquad \|Df_{|E^s_x}\| \left\| Df^{-1}_{|E^c_{f^{-1}(x)}} \right\| < \gamma \quad \forall x \in \Lambda.$$

There exists many different constructions of robustly transitive partial hyperbolic systems. We list some of them: Product and Skew products of a hyperbolic system with a non-hyperbolic one; Bifurcation of Anosov maps or maps isotopic to an Anosov system; Time one map of an Anosov flow; Toral automorphisms with some hyperbolic subbundles; Partially hyperbolic affine diffeomorphisms of finite volume compact homogeneous spaces of simple Lie groups.

Now we are going to describe some of them that has relevant connotations in symplectic dynamics. In this context, the theory of Kolmogorov, Arnold and Moser, (KAM) gives a precise description of the dynamics of a set of large measure of orbits for any small perturbation of a non-degenerate integrable Hamiltonian system. These orbits lie on the invariant KAM tori for which the dynamics are equivalent to irrational (Diophantine) rotations. This theory applies for the autonomous Hamiltonians, time-periodic Hamiltonians and also for symplectic diffeomorphisms.

In the case of autonomous systems in two degrees of freedom or time-periodic systems in one degree of freedom (i.e., 1.5 degrees of freedom), the KAM theorem proves the stability of *all* orbits, in the sense that the actions do not vary much along the orbits. Since each KAM torus has codimension one in the phase space, its complement is disconnected and contains two connected invariant components. Thus, any orbit remains between two nearby invariant tori. This, of course, is not

the case if the degree of freedom is larger than two, where the KAM tori are of codimension at least two. A natural question arises: Do generic perturbations of integrable systems in higher dimensions exhibit instabilities?

The problem of instabilities for high dimensional nearly integrable Hamiltonian systems (i.e. small perturbations of integrable systems) has been considered one of the most important problems in Hamiltonian dynamics. The first example of instability is due to Arnold [6], who constructed a family of small perturbations of a non-degenerate integrable Hamiltonian system that exhibits instability in the sense that there are orbits for which the variation of action is large. This kind of topological instability is sometimes called the *Arnold diffusion*. In fact, he had conjectured [7, pp. 176] that the answer of the above question should be positive. While there is a large number of works and announcements towards this conjecture, specially in the recent years (see e.g. [19, 26, 22, 33, 34, 54], and references there), little is known about "most of the orbits" in the complement of invariant or periodic Diophantine tori. Although it is very difficult to prove the existence of "some" instable orbits in general, it is the simplest expected non-trivial behavior in the complement of invariant tori. For instance, one may ask about transitivity or topological mixing.

A goal therefore, is to study the dynamics in the complement of invariant KAM tori with a focus on the non-local robust phenomena, mainly robust transitivity and robust topological mixing. In particular, the methods of robust transitivity and partially hyperbolicity can be developed into the context of symplectic and Hamiltonian systems, and apply them for the nearly integrable symplectic and Hamiltonian systems with more than two degrees of freedom. This allows to introduce Hamiltonians or symplectic diffeomorphisms exhibiting *unbounded or large* robustly transitive sets. Then, the instability (or the so-called Arnold diffusion) is obtained as a consequence of the existence of large or unbounded robustly transitive sets. In particular, theorem A in [40], says:

> *If the product of a hyperbolic basic set Λ by any non-wandering dynamics on N is partially hyperbolic then we can perturb it in such a way that (the continuation of) $\Lambda \times N$ become a robustly topological mixing set.*

To exemplify this, consider a product of a hyperbolic set (for instance a horseshoes) by a Twist map. Similar results can be stated in the context of exact and Hamiltonian diffeomorphisms, and also time-dependent Hamiltonians. These results concern the class of integrable systems that contains the so-called *a priori* unstable integrable Hamiltonian systems H (cf. [19, 22, 54]).

2.3 Dominated Splitting

There is also another category which includes the partially hyperbolic system: *dominated splitting*. An f-invariant set Λ is said to have dominated splitting if we can decompose its tangent bundle in two invariant subbundles $T_\Lambda M = E \oplus F$, such that:

$$\|Df^n_{/E(x)}\| \|Df^{-n}_{/F(f^n(x))}\| \leq C\lambda^n, \quad \text{for all } x \in \Lambda, n \geq 0$$

with $C > 0$ and $0 < \lambda < 1$. Of course, it is assumed that neither of the subbundless is trivial (otherwise, the other one has a uniform hyperbolic behavior: contracting or expanding).

Let us explain briefly the meaning of the above definition: it says that, for n large, the "greatest expansion" of Df^n on E is less than the "greatest contraction" of Df^n on F and by a factor that becomes exponentially small with n. In other words, every direction not belonging to E must converge exponentially fast under iteration of Df to the direction F. This notion was first introduced independently by Mañé, Liao, and Pliss, as a first step in the attempt to prove that structurally stable systems satisfy a hyperbolic condition on the tangent map. Simple examples of invariant sets exhibiting dominated splitting which are not hyperbolic splitting are normally hyperbolic closed invariant curves with dynamics conjugate to irrational rotations and homoclinic classes associated to non-hyperbolic fixed points. These examples are not robustly transitive. However, as it was said in the introduction, in [15] it was proved that in dimension larger and equal than four there are robustly transitive diffeomorphisms exhibiting a dominated splitting which have no expanding or contracting invariant sub-bundle therefore, they are neither hyperbolic nor partially hyperbolic. See [15, 18, 47, 49] for references about this constructions.

To explain a natural framework, where the dominated splitting dynamics appears, we have to recall a natural generalization of a Riemann manifold which are the Weyl structure. It is a torsion free connection whose parallel transport preserves a given conformal class of metrics. We follow the work and exposition of Maciej P. Wojtkowski [53] to describe the interplay between a Weyl manifold, a Weyl flow, a Gaussian thermostat, and a dominated splitting.

Fixed a Riemannian metric $\langle , \rangle$, let ∇ be the Levi-Civita connection, and let E be a vector field. Define the connection $\hat{\nabla}$ as

$$\hat{\nabla}_X Y = \nabla_X Y + \langle X, E\rangle Y + \langle Y, E\rangle X - \langle X, Y\rangle E;$$

where X, Y denote arbitrary vector fields. The geodesics of the Weyl connection are given by the equations in TM

$$\frac{\partial q}{\partial s} = w, \quad \frac{\hat{D}w}{\partial s} = 0$$

where $\frac{\hat{D}w}{\partial s}$ denotes the covariant derivative $\hat{\nabla}_w$. These equations provide geodesics with a distinguished parameter s, unique up to scale. The W-flow $\Phi_t : SM \to SM$ is obtained by parameterizing the geodesics of the Weyl connection with the arc length of g.

There are examples that reveals a major departure from geodesic flows and Hamiltonian dynamics (see [53]): W-flows may contract phase volume and they may have no absolutely continuous invariant measure; in particular, they can exhibit attractors.

The curvature tensor can be defined and therefore the sectional curvature. The next theorem (see [53]) is similar to the one obtained for geodesic flows on manifolds of negative curvature, replacing hyperbolicity by a dominated splitting:

> *If the sectional curvatures of the Weyl structure are negative everywhere in M then the W-flow has a dominated splitting $E \oplus F$ such that the flow shows exponential growth of volume in F and exponential decay of volume in E.*

Moreover, in [53], Wojtkowski conjectured that there are three-dimensional manifolds and vector fields such that the sectional curvatures of the corresponding Weyl structure are negative but the W-flow is not Anosov neither partially hyperbolic. In this context, the construction performed in [15] could play an important role.

Such W-flows turn out to have a natural physical interpretation: they are identical to Gaussian thermostats, or isokinetic dynamics, introduced by Hoover in [30]. Isokinetic dynamics provides useful models in nonequilibrium statistical mechanics, discussed in the papers of Gallavotti and Ruelle, [27, 51, 28].

2.4 A General Question About "Weak Form of Hyperbolicity"

One of the reason of the success of hyperbolic dynamics follows from the fact that under the assumption of hyperbolicity one obtains a satisfactory (complete) description of the dynamics of the system from a topological and statistical point of view. One example of this is the well known spectral decomposition theorem for hyperbolic systems: Under the assumption that the nonwandering set is hyperbolic and the periodic points are dense, Smale proved that the nonwandering set can be decomposed into the disjoint union of finitely compact invariant and transitive sets.

This is far from be true in the case of partially hyperbolic dynamics and dominated splitting. To give an example of that, let us consider the following result easily obtained in the case of hyperbolic dynamics: *A transitive Anosov diffeomorphism is C^r robust transitive*. A similar statement is false both in the case of partially hyperbolic dynamics and dominated splitting. Therefore, the natural question arise:

> *Can we characterize robust transitive partially hyperbolic dynamics*? *Can we characterize robust transitive dynamics exhibiting dominated splitting*?

Regarding the type of structure that robust transitive systems exhibit and describe in Sect. 2, answering previous question would be essential to have a complete description of C^1 robust transitive systems.

2.5 Robust Transitivity and Mechanisms: Heterodimensional Cycle

As we said in the introduction, one of the goals in the theory of robust transitivity, is to understand which is the mechanisms underlying the robustness. Here, we are going to summarize the role played, in the robust transitivity, by a type of bifurcation called heterodimensional cycles (see [24, 23]). More precisely:

Let $f \in \mathrm{Diff}^r(M)$ $(r \geq t1)$. Let us assume that f has a pair of hyperbolic saddles P and Q with different indices, that is, different dimensions of their unstable subspaces. Assume $W^s(P)$ and $W^u(Q)$ have non-empty intersection, and the same for $W^u(P)$ and $W^s(Q)$. We say that f has a **heterodimensional cycle** *associated to P and Q.*

It follows immediately from the definition that heterodimensional cycles can only exist in dimension bigger or equal to 3. The main result about this bifurcation, can be summarize in the following theorem

Let $f \in \mathrm{Diff}^1(M)$ and $\Lambda_f(U) = \bigcap_{\{n\in\mathbb{Z}\}} g^n(U)$ be a maximal invariant nonhyperbolic C^1-robust transitive sets. Then, there is g C^1-close to f such that g exhibits a heterodimensional cycles contained in $\Lambda_g(U) = \bigcap_{\{n\in\mathbb{Z}\}} g^n(U)$.

In the same sense, these cycles play the role for the partial hyperbolic theory as transverse intersection play for the hyperbolic theory. In the paper [16] is studied the interplay done between heterodimensional cycles and robust transitive systems in any dimension.

To show the richness of the heterodimensional cycles we will expose one theorem related to them. The next theorem asserts that given a heterodimensional cycle, the homoclinic classes obtained after the bifurcation of the cycle often explode, and become intermingled (non-empty intersection) when the cycle is unfolded ([24]):

Let $f \in \mathrm{Diff}^1(M^n)$ exhibiting a heterodimensional cycle associated to two fixed points p and q. Then, there is a small neighborhood U containing p and q and g C^1 arbitrarily close to f such that $\Lambda_g(U)$ a maximal invariant nonhyperbolic C^1-robust transitive sets.

3 Wild Dynamics

Recall that with wild diffeomorphisms, it is called a diffeomorphisms having infinitely many isolated transitive sets such that the same holds for a residual set of perturbation of it. The first examples of wild dynamics were discovered by Newhouse, in the setting of C^2 surface diffeomorphisms. He proved that there exist an open subset U of $\mathrm{Diff}^r(M)$, $r \geq 2$, and a residual subset in U consisting of diffeomorphisms with infinitely many sinks or sources. As we mentioned before, this construction is intimately associated to homoclinic phenomena.

3.1 Wild Dynamic and Homoclinic Tangency

In this section we will mention some of the dynamical phenomena related to the presences of homoclinic tangencies. For that, first we recall that the stable and unstable sets

$$W^s(p) = \{y \in M : \mathrm{dist}(f^n(y), f^n(p)) \to 0 \text{ as } n \to \infty\},$$
$$W^u(p) = \{y \in M : \mathrm{dist}(f^n(y), f^n(p)) \to 0 \text{ as } n \to -\infty\}$$

are C^r-injectively immersed submanifolds when p is a hyperbolic periodic point of f.

Given $f : M \to M$ a diffeomorphism, it is said that f exhibits a homoclinic tangency if there is a hyperbolic periodic point p of f such that the stable and unstable manifolds of p have a non-transverse intersection.

It is important to say that a homoclinic tangency is (locally) easily destroyed by small perturbation of the invariant manifolds. To get open sets of diffeomorphisms where each system exhibits an homoclinic tangency, Newhouse study system where the homoclinic tangency is associated to an invariant hyperbolic set with the property that it has large fractal dimension (here is important to remark that his construction only works in the C^2 topology).

Other fundamental dynamic prototypes were found in the context of this bifurcation, namely the so called cascade of bifurcations, the Hénon-like strange attractor ([9, 37]) (infinitely many coexisting ones [20]), and super exponential growth of periodic points ([32]).

Nevertheless the rich dynamics that appear after the unfolding of an homoclinic tangency, Palis conjectured (see [44]) that for a generic one parameter family of surfaces maps unfolding a homoclinic tangency, the set of parameter values corresponding to diffeomorphisms with infinitely many sinks or infinitely many Hénon-like attractors has (Lebesgue) measure zero.

In this direction in [46] is announced that given a surface diffeomorphisms f_0 such that the maximal invariant set in an open set V is the union of a horseshoe and a quadratic tangency between the stable and unstable foliations of this horseshoe such that the dimension of the horseshoe is larger than but close to one, then for most diffeomorphisms f close to f_0, the maximal f-invariant set in V is a non-uniformly hyperbolic horseshoe, with dynamics of the same type as met in Henon attractors. In particular, most diffeomorphisms (in a measure theoretical point of view for parameters in one-parameter families) does not exhibit attracting periodic points.

In higher dimension, many of the previous result were generalized (see [45, 51, 39]).

As it was mentioned at the beginning when we referred to the Newhouse's techniques, all the previous results hold when are considered at least C^2 diffeomorphisms. However, in [14] was obtained the (coexistence of infinitely many sinks or sources) for C^1 diffeomorphisms on three dimensional manifolds.

3.2 Surfaces Diffeomorphisms and Beyond

The presence of homoclinic tangencies have many analogies with the presence of critical points for one-dimensional endomorphisms. On one hand, homoclinic tangencies correspond in the one dimensional setting to preperiodic critical points and it is known that its bifurcation leads to complex dynamics. On the other hand, Mañé (see [36]) showed that for regular and generic one-dimensional endomorphisms, the

absence of critical points is enough to guarantee hyperbolicity. This result raises the question about the dynamical properties of surface maps exhibiting no homoclinic tangencies. As dominated splitting prevents the presence of tangencies, we could say that domination plays for surface diffeomorphisms the role that the non critical behavior does for one dimensional endomorphisms.

One may ask whether a set having dominated splitting is hyperbolic. Two necessary conditions follows trivially: all the periodic points in the set must be hyperbolic and no attracting (repelling) closed invariant (periodic) curve supporting an irrational rotation is in the set.

The next result says that these two conditions are also sufficient as long as the diffeomorphism is smooth enough. It is the analogous of a one dimensional theorem by Mañe (see [36, 48, 50]).

> *Let $f \in \mathrm{Diff}^2(M^2)$ and assume that $\Lambda \subset \Omega(f)$ is a compact invariant set exhibiting a dominated splitting such that any periodic point in Λ is hyperbolic. Then, $\Lambda = \Lambda_1 \cup \Lambda_2$ where Λ_1 is a hyperbolic set and Λ_2 consists of a finite union of periodic simple closed curves $\mathscr{C}_1, \ldots, \mathscr{C}_n$, normally hyperbolic, and such that $f^{m_i} : \mathscr{C}_i \to \mathscr{C}_i$ is conjugated to an irrational rotation (m_i denotes the period of $\mathscr{C}_i$).*

This result, permit to prove the following theorem which describes the C^1 generic dynamics in terms of Palis's conjecture stated in next section:

> *Let $f \in \mathrm{Diff}^2(M^2)$ be C^1 far from tangencies. Then, f can be C^1 approximated by an Axiom A diffeomorphism.*

Moreover, it is possible to relate wild dynamics with the unfolding of homoclinic tangencies:

> *Let $f \in \mathrm{Diff}^2(M^2)$ have infinitely many sinks or sources with unbounded period. Then, f can be C^1 approximated by a diffeomorphism exhibiting a homoclinic tangency.*

The previous results are false in higher dimension due to the existence of robust transitive diffeomorphisms with partially hyperbolic splitting.

4 Generic Dynamics: Mechanisms and Phenomenas

Two basic mechanisms were found to the obstruction of hyperbolicity, are *heterodimensional cycles* and *homoclinic tangencies*. In fact, as we described in Sect. 2.5, heterodimensional cycle are the core mechanisms for robust non-hyperbolic dynamics and tangencies are generating wild dynamics (recall Sect. 3). Addressing this remark, in the early 80's Palis conjectured that these are very common in the complement of the hyperbolic systems:

Palis'Conjecture:

1. *Every C^r diffeomorphism of a compact manifold M can be C^r approximated by one which is hyperbolic or by one exhibiting a heterodimensional cycle or by one exhibiting a homoclinic tangency.*
2. *When M is a two-dimensional compact manifold every C^r diffeomorphism of M can be C^r approximated by one which is hyperbolic or by one exhibiting a homoclinic tangency.*

This conjecture may be thought as a start point to obtaining a generic description of C^r diffeomorphisms. If it turns out to be true, we may focus on the two mechanisms mentioned above in order to understand the dynamics. Nevertheless, the unfolding of these homoclinic bifurcations is still mainly a local study.

For the case of surfaces and the C^1 topology, the theorem A in [48] proves the conjecture. When the manifold has dimension greater than two the main result in this direction is the following one proved in [21].

> *Any* $f \in \mathrm{Diff}^1(M)$ *can be* C^1*-approximated by another diffeomorphism such that either*
>
> 1. *it has a homoclinic tangency or,*
> 2. *it has a heterodimensional cycle or,*
> 3. *it is essentially hyperbolic.*

Given $f \in \mathrm{Diff}^1(M)$, it is said that f is *essentially hyperbolic if there exists a finite number of transitive hyperbolic attractors such that the union of their basins of attraction are open and dense.*

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Dynamics of Bose-Einstein Condensates

Benjamin Schlein

Abstract We report on some recent results concerning the dynamics of Bose-Einstein condensates, obtained in a series of joint papers [7, 8] with L. Erdős and H.-T. Yau. Starting from many body quantum dynamics, we present a rigorous derivation of a cubic nonlinear Schrödinger equation known as the Gross-Pitaevskii equation for the time evolution of the condensate wave function.

1 Introduction

Bosonic systems at very low temperature are characterized by the fact that a macroscopic fraction of the particles collapses into a single one-particle state. Although this phenomenon, known as Bose-Einstein condensation, was already predicted in the early days of quantum mechanics, the first empirical evidence for its existence was only obtained in 1995, in experiments performed by groups led by Cornell and Wieman at the University of Colorado at Boulder and by Ketterle at MIT (see [2, 4]). In these important experiments, atomic gases were initially trapped by magnetic fields and cooled down at very low temperatures. Then the magnetic traps were switched off and the consequent time evolution of the gas was observed; for sufficiently small temperatures, the particles remained close together and the gas moved as a single particle, a clear sign for the existence of condensation.

In the last years important progress has also been achieved in the theoretical understanding of Bose-Einstein condensation. In [10], Lieb, Seiringer, and Yngvason considered a trapped Bose gas consisting of N three-dimensional particles described by the Hamiltonian

Benjamin Schlein
DPMMS, University of Cambridge, Wilberforce Rd., Cambridge, CB3 0WB, UK

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$$H_N^{\text{trap}} = \sum_{j=1}^{N} \big(-\Delta_j + V_{\text{ext}}(x_j)\big) + \sum_{i<j}^{N} V_a(x_i - x_j) \tag{1}$$

where V_{ext} is an external confining potential and $V_a(x)$ is a repulsive interaction potential with scattering length a (here and in the rest of the paper we use the notation $\nabla_j = \nabla_{x_j}$ and $\Delta_j = \Delta_{x_j}$). Letting $N \to \infty$ and $a \to 0$ with $Na = a_0$ fixed, they showed that the ground state energy $E(N)$ of (1) divided by the number of particle N converges to

$$\lim_{N\to\infty,\ Na=a_0} \frac{E(N)}{N} = \min_{\varphi\in L^2(\mathbb{R}^3):\ \|\varphi\|=1} \mathscr{E}_{\text{GP}}(\varphi)$$

where $\mathscr{E}_{\text{GP}}$ is the Gross-Pitaevskii energy functional

$$\mathscr{E}_{\text{GP}}(\varphi) = \int \mathrm{d}x\, (|\nabla\varphi(x)|^2 + V_{\text{ext}}(x)|\varphi(x)|^2 + 4\pi a_0 |\varphi(x)|^4). \tag{2}$$

Later, in [9], Lieb and Seiringer also proved that trapped Bose gases characterized by the Gross-Pitaevskii scaling $Na = a_0 = \text{const}$ exhibit Bose-Einstein condensation in the ground state. More precisely, they showed that, if ψ_N is the ground state wave function of the Hamiltonian (1) and if $\gamma_N^{(1)}$ denotes the corresponding one-particle marginal (defined as the partial trace of the density matrix $\gamma_N = |\psi_N\rangle\langle\psi_N|$ over the last $N-1$ particles, with the convention that $\text{Tr}\,\gamma_N^{(1)} = 1$ for all N), then

$$\gamma_N^{(1)} \to |\phi_{\text{GP}}\rangle\langle\phi_{\text{GP}}| \quad \text{as } N \to \infty. \tag{3}$$

Here $\phi_{\text{GP}} \in L^2(\mathbb{R}^3)$ is the minimizer of the Gross-Pitaevskii energy functional (2). The interpretation of this result is straightforward; in the limit of large N, all particles, apart from a fraction vanishing as $N \to \infty$, are in the same one-particle state described by the wave-function $\phi_{\text{GP}} \in L^2(\mathbb{R}^3)$. In this sense the ground state of (1) exhibits complete Bose-Einstein condensation into ϕ_{GP}.

In joint works with L. Erdős and H.-T. Yau (see [7, 8, 6]), we prove that the Gross-Pitaevskii theory can also be used to describe the dynamics of Bose-Einstein condensates. In the Gross-Pitaevskii scaling (characterized by the fact that the scattering length of the interaction potential is of the order $1/N$) we show, under some conditions on the interaction potential and on the initial N-particle wave function, that complete Bose-Einstein condensation is preserved by the time evolution. Moreover we prove that the dynamics of the condensate wave function is governed by the time-dependent Gross-Pitaevskii equation associated with the energy functional (2).

As an example, consider the experimental set-up described above, where the dynamics of an initially confined gas is observed after removing the traps. Mathematically, the trapped gas can be described by the Hamiltonian (1), where the confining potential V_{ext} models the magnetic traps. When cooled down at very low temperatures, the system essentially relaxes to the ground state ψ_N of (1); from [9] it follows that at time $t = 0$, immediately before switching off the traps, the system exhibits

complete Bose-Einstein condensation into $\phi_{\rm GP}$ in the sense (3). At time $t = 0$ the traps are turned off, and one observes the evolution of the system generated by the translation invariant Hamiltonian

$$H_N = -\sum_{j=1}^{N} \Delta_j + \sum_{i<j}^{N} V_a(x_i - x_j).$$

Our results (stated in more details in Sect. 3 below) imply that, if $\psi_{N,t} = e^{-iH_N t}\psi_N$ is the time evolution of the initial wave function ψ_N and if $\gamma^{(1)}_{N,t}$ denotes the one-particle marginal associated with $\psi_{N,t}$, then, for any fixed time $t \in \mathbb{R}$,

$$\gamma^{(1)}_{N,t} \to |\varphi_t\rangle\langle\varphi_t| \qquad \text{as } N \to \infty$$

where φ_t is the solution of the nonlinear time-dependent Gross-Pitaevskii equation

$$i\partial_t \varphi_t = -\Delta\varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t \tag{4}$$

with the initial data $\varphi_{t=0} = \phi_{\rm GP}$. In other words, we prove that at arbitrary time $t \in \mathbb{R}$, the system still exhibits complete condensation, and the time-evolution of the condensate wave function is determined by the Gross-Pitaevskii equation (4).

The goal of this manuscript is to illustrate the main ideas of the proof of the results obtained in [7, 8, 6]. The paper is organized as follows. In Sect. 2 we define the model more precisely, and we give a heuristic argument to explain the emergence of the Gross-Pitaevskii equation (4). In Sect. 3 we present our main results. In Sect. 4 we illustrate the general strategy used to prove the main results and, finally, in Sects. 5 and 6 we discuss the two most important parts of the proof in some more details.

2 Heuristic Derivation of the Gross-Pitaevskii Equation

To describe the interaction among the particles we choose a positive, spherical symmetric, compactly supported, smooth function $V(x)$. We denote the scattering length of V by a_0.

Recall that the scattering length of V is defined by the spherical symmetric solution to the zero energy equation

$$\left(-\Delta + \frac{1}{2}V(x)\right) f(x) = 0 \quad f(x) \to 1 \text{ as } |x| \to \infty. \tag{5}$$

The scattering length of V is defined then by

$$a_0 = \lim_{|x|\to\infty} |x| - |x| f(x).$$

This limit can be proven to exist if V decays sufficiently fast at infinity. Note that, since we assumed V to have compact support, we have

$$f(x) = 1 - \frac{a_0}{|x|} \tag{6}$$

for $|x|$ sufficiently large. Another equivalent characterization of the scattering length is given by

$$8\pi a_0 = \int \mathrm{d}x\, V(x) f(x). \tag{7}$$

To recover the Gross-Pitaevskii scaling, we define $V_N(x) = N^2 V(Nx)$. By scaling it is clear that the scattering length of V_N equals $a = a_0/N$. In fact if $f(x)$ is the solution to (5), it is clear that $f_N(x) = f(Nx)$ solves

$$\left(-\Delta + \frac{1}{2} V_N(x)\right) f_N(x) = 0 \tag{8}$$

with the boundary condition $f_N(x) \to 1$ as $|x| \to \infty$. From (6), we obtain

$$f_N(x) = 1 - \frac{a_0}{N|x|} = 1 - \frac{a}{|x|}$$

for $|x|$ large enough. In particular the scattering length a of V_N is given by $a = a_0/N$.

We consider the dynamics generated by the translation invariant Hamiltonian

$$H_N = \sum_{j=1}^{N} -\Delta_j + \sum_{i<j}^{N} V_N(x_i - x_j) \tag{9}$$

acting on the Hilbert space $L^2_s(\mathbb{R}^{3N}, \mathrm{d}x_1 \cdots \mathrm{d}x_N)$, the bosonic subspace of $L^2(\mathbb{R}^{3N}, \mathrm{d}x_1 \cdots \mathrm{d}x_N)$ consisting of all permutation symmetric functions (although it is possible to extend our analysis to include an external potential, to keep the discussion as simple as possible we only consider the translation invariant case (9)). We consider solutions $\psi_{N,t}$ of the N-body Schroedinger equation

$$i\partial_t \psi_{N,t} = H_N \psi_{N,t}. \tag{10}$$

Let $\gamma_{N,t} = |\psi_{N,t}\rangle\langle\psi_{N,t}|$ denote the density matrix associated with $\psi_{N,t}$, defined as the orthogonal projection onto $\psi_{N,t}$. In order to study the limit $N \to \infty$, we introduce the marginal densities of $\gamma_{N,t}$. For $k = 1, \ldots, N$, we define the k-particle density matrix $\gamma^{(k)}_{N,t}$ associated with $\psi_{N,t}$ by taking the partial trace of $\gamma_{N,t}$ over the last $N - k$ particles. In other words, $\gamma^{(k)}_{N,t}$ is defined as the positive trace class operator on $L^2_s(\mathbb{R}^{3k})$ with kernel given by

$$\gamma^{(k)}_{N,t}(\mathbf{x}_k; \mathbf{x}'_k) = \int \mathrm{d}\mathbf{x}_{N-k}\, \psi_{N,t}(\mathbf{x}_k, \mathbf{x}_{N-k}) \overline{\psi}_{N,t}(\mathbf{x}'_k, \mathbf{x}_{N-k}). \tag{11}$$

Here and in the rest of the paper we use the notation $\mathbf{x} = (x_1, x_2, \dots, x_N)$, $\mathbf{x}_k = (x_1, x_2, \dots, x_k)$, $\mathbf{x}'_k = (x'_1, x'_2, \dots, x'_k)$, and $\mathbf{x}_{N-k} = (x_{k+1}, x_{k+2}, \dots, x_N)$.

We consider initial wave functions $\psi_{N,0}$ exhibiting complete condensation in a one-particle state φ. Thus at time $t = 0$, we assume that

$$\gamma^{(1)}_{N,0} \to |\varphi\rangle\langle\varphi| \qquad \text{as } N \to \infty. \tag{12}$$

It turns out that the last equation immediately implies that

$$\gamma^{(k)}_{N,0} \to |\varphi\rangle\langle\varphi|^{\otimes k} \qquad \text{as } N \to \infty \tag{13}$$

for every fixed $k \in \mathbb{N}$ (the argument, due to Lieb and Seiringer, can be found in [9], after Theorem 1). It is also interesting to notice that the convergence (12) (and (13)) in the trace class norm is equivalent to the convergence in the weak* topology defined on the space of trace class operators on $\mathbb{R}^3$ (or $\mathbb{R}^{3k}$, for (13)); we thank A. Michelangeli for pointing out this fact to us (the proof is based on general arguments, such as Grümm's Convergence Theorem).

Starting from the Schroedinger equation (10) for the wave function $\psi_{N,t}$, we can derive evolution equations for the marginal densities $\gamma^{(k)}_{N,t}$. The dynamics of the marginals is governed by a hierarchy of N coupled equations usually known as the BBGKY hierarchy,

$$\begin{aligned} i\partial_t \gamma^{(k)}_{N,t} = &\sum_{j=1}^{N} \left[-\Delta_j, \gamma^{(k)}_{N,t}\right] + \sum_{i<j}^{k} \left[V_N(x_i - x_j), \gamma^{(k)}_{N,t}\right] \\ &+ (N-k) \sum_{j=1}^{k} \mathrm{Tr}_{k+1}\left[V_N(x_j - x_{k+1}), \gamma^{(k+1)}_{N,t}\right]. \end{aligned} \tag{14}$$

Here Tr_{k+1} denotes the partial trace over the $(k+1)$-th particle.

Next we study the limit $N \to \infty$ of the density $\gamma^{(k)}_{N,t}$ for fixed $k \in \mathbb{N}$. For simplicity we fix $k = 1$. From (14), the evolution equation for the one-particle density matrix, written in terms of its kernel $\gamma^{(1)}_{N,t}(x_1; x'_1)$ is given by

$$\begin{aligned} &i\partial_t \gamma^{(1)}_{N,t}(x_1, x'_1) \\ &\quad = (-\Delta_1 + \Delta'_1)\gamma^{(1)}_{N,t}(x_1; x'_1) \\ &\qquad + (N-1) \int \mathrm{d}x_2 (V_N(x_1 - x_2) - V_N(x'_1 - x_2))\gamma^{(2)}_{N,t}(x_1, x_2; x'_1, x_2). \end{aligned} \tag{15}$$

Suppose now that $\gamma^{(1)}_{\infty,t}$ and $\gamma^{(2)}_{\infty,t}$ are limit points (with respect to the weak* topology) of $\gamma^{(1)}_{N,t}$ and, respectively, $\gamma^{(2)}_{N,t}$ as $N \to \infty$. Since, formally,

$$(N-1)V_N(x) = (N-1)N^2 V(Nx) \simeq N^3 V(Nx) \to b_0 \delta(x)$$

with $b_0 = \int \mathrm{d}x\, V(x)$ as $N \to \infty$, we could naively expect the limit points $\gamma^{(1)}_{\infty,t}$ and $\gamma^{(2)}_{\infty,t}$ to satisfy the limiting equation

$$\begin{aligned} i\partial_t \gamma^{(1)}_{\infty,t}(x_1; x_1') &= (-\Delta_1 + \Delta_1')\gamma^{(1)}_{\infty,t}(x_1; x_1') \\ &\quad + b_0 \int \mathrm{d}x_2 (\delta(x_1 - x_2) - \delta(x_1' - x_2))\gamma^{(2)}_{\infty,t}(x_1, x_2; x_1', x_2). \end{aligned} \tag{16}$$

From (13) we have, at time $t = 0$,

$$\begin{aligned} \gamma^{(1)}_{\infty,0}(x_1; x_1') &= \varphi(x_1)\overline{\varphi}(x_1') \\ \gamma^{(2)}_{\infty,0}(x_1, x_2; x_1', x_2') &= \varphi(x_1)\varphi(x_2)\overline{\varphi}(x_1')\overline{\varphi}(x_2'). \end{aligned} \tag{17}$$

If condensation is really preserved by the time evolution, also at time $t \neq 0$ we have

$$\begin{aligned} \gamma^{(1)}_{\infty,t}(x_1; x_1') &= \varphi_t(x_1)\overline{\varphi}_t(x_1') \\ \gamma^{(2)}_{\infty,t}(x_1, x_2; x_1', x_2') &= \varphi_t(x_1)\varphi_t(x_2)\overline{\varphi}_t(x_1')\overline{\varphi}_t(x_2'). \end{aligned} \tag{18}$$

Inserting (18) in (16), we obtain the self-consistent equation

$$i\partial_t \varphi_t = -\Delta\varphi_t + b_0|\varphi_t|^2\varphi_t \tag{19}$$

for the condensate wave function φ_t. This equation has the same form as the time-dependent Gross-Pitaevskii equation (4), but a different coefficient in front of the nonlinearity (b_0 instead of $8\pi a_0$).

The reason why we obtain the wrong coupling constant in (19) is that going from (15) to (16), we took the two limits

$$(N-1)V_N(x) \to b_0\delta(x) \quad \text{and} \quad \gamma^{(2)}_{N,t} \to \gamma^{(2)}_{\infty,t} \tag{20}$$

independently from each other. However, since the scattering length of the interaction is of the order $1/N$, the two-particle density $\gamma^{(2)}_{N,t}$ develops a short scale correlation structure on the length scale $1/N$, which is exactly the same length scale on which the potential V_N varies. For this reason the two limits in (20) cannot be taken independently. In order to obtain the correct Gross-Pitaevskii equation (4) we need to take into account the correlations among the particles, and the short scale structure they create in the marginal density $\gamma^{(2)}_{N,t}$.

To describe the correlations among the particles we make use of the solution $f_N(x)$ to the zero energy scattering equation (8). Assuming that the function $f_N(x_i - x_j)$ gives a good approximation for the correlations between particles i and j, we may expect that the one- and two-particle densities associated with the evolution of a condensate are given, for large but finite N, by

$$\begin{aligned} \gamma^{(1)}_{N,t}(x_1; x_1') &\simeq \varphi_t(x_1)\overline{\varphi}_t(x_1') \\ \gamma^{(2)}_{N,t}(x_1, x_2; x_1', x_2') &\simeq f_N(x_1 - x_2) f_N(x_1' - x_2')\varphi_t(x_1)\varphi_t(x_2)\overline{\varphi}_t(x_1')\overline{\varphi}_t(x_2'). \end{aligned} \tag{21}$$

Inserting this ansatz into (15), we obtain a new self-consistent equation

$$\begin{aligned} i\partial_t\varphi_t &= -\Delta\varphi_t + \left(\lim_{N\to\infty}(N-1)\int \mathrm{d}x f_N(x)V_N(x)\right)|\varphi_t|^2\varphi_t \\ &= -\Delta\varphi_t + \left(\lim_{N\to\infty} N^3\int \mathrm{d}x f(Nx)V(Nx)\right)|\varphi_t|^2\varphi_t \\ &= -\Delta\varphi_t + 8\pi a_0|\varphi_t|^2\varphi_t \end{aligned} \tag{22}$$

because of (7). This is exactly the Gross-Pitaevskii equation (4), with the correct coupling constant in front of the nonlinearity.

Note that the presence of the correlation functions $f_N(x_1 - x_2)$ and $f_N(x_1' - x_2')$ in (21) does not contradict complete condensation of the system at time t. On the contrary, in the weak limit $N \to \infty$, the function f_N converges to one, and therefore $\gamma^{(1)}_{N,t}$ and $\gamma^{(2)}_{N,t}$ converge to $|\varphi_t\rangle\langle\varphi_t|$ and $|\varphi_t\rangle\langle\varphi_t|^{\otimes 2}$, respectively. The correlations described by the function f_N can only produce nontrivial effects on the macroscopic dynamics of the system because of the singularity of the interaction potential V_N.

From this heuristic argument it is clear that, in order to obtain a rigorous derivation of the Gross-Pitaevskii equation (22), we need to identify the short scale structure of the marginal densities and prove that, in a very good approximation, it can be described by the function f_N as in (21). In other words, we need to show a very strong separation of scales in the marginal density $\gamma^{(2)}_{N,t}$ (and, more generally, in the k-particle density $\gamma^{(k)}_{N,t}$) associated with the solution of the N-body Schrödinger equation; the Gross-Pitaevskii theory can only be correct if $\gamma^{(k)}_{N,t}$ has a regular part, which factorizes for large N into the product of k copies of the orthogonal projection $|\varphi_t\rangle\langle\varphi_t|$, and a time independent singular part, due to the correlations among the particles, and described by products of the functions $f_N(x_i - x_j)$, $1 \le i, j \le k$.

3 Main Results

To prove our main results we need to assume the interaction potential to be sufficiently weak. To measure the strength of the potential, we introduce the dimensionless quantity

$$\alpha = \sup_{x\in\mathbb{R}^3} |x|^2 V(x) + \int \frac{\mathrm{d}x}{|x|} V(x). \tag{23}$$

Apart from the smallness assumption on the potential, we also need to assume that the correlations characterizing the initial N-particle wave function are sufficiently weak. We define therefore the notion of *asymptotically factorized* wave functions. We say that a family of permutation symmetric wave functions ψ_N is asymptotically factorized if there exists $\varphi \in L^2(\mathbb{R}^3)$ and, for any fixed $k \ge 1$, there exists a family $\xi_N^{(N-k)} \in L^2_s(\mathbb{R}^{3(N-k)})$ such that

$$\left\| \psi_N - \varphi^{\otimes k} \otimes \xi_N^{(N-k)} \right\| \to 0 \qquad \text{as } N \to \infty. \tag{24}$$

It is simple to check that, if ψ_N is asymptotically factorized, then it exhibits complete Bose-Einstein condensation in the one-particle state φ (in the sense that the one-particle density associated with ψ_N satisfy $\gamma_N^{(1)} \to |\varphi\rangle\langle\varphi|$ as $N \to \infty$). Asymptotic factorization is therefore a stronger condition than complete condensation, and it provides more control on the correlations of ψ_N.

Theorem 1. *Assume that $V(x)$ is a positive, smooth, spherical symmetric, and compactly supported potential such that α (defined in (23)) is sufficiently small. Consider an asymptotically factorized family of wave functions $\psi_N \in L^2_s(\mathbb{R}^{3N})$, exhibiting complete Bose-Einstein condensation in a one-particle state $\varphi \in H^1(\mathbb{R}^3)$, in the sense that*

$$\gamma_N^{(1)} \to |\varphi\rangle\langle\varphi| \quad \text{as } N \to \infty \tag{25}$$

where $\gamma_N^{(1)}$ denotes the one-particle density associated with ψ_N. Then, for any fixed $t \in \mathbb{R}$, the one-particle density $\gamma_{N,t}^{(1)}$ associated with the solution $\psi_{N,t}$ of the N-particle Schrödinger equation (10) satisfies

$$\gamma_{N,t}^{(1)} \to |\varphi_t\rangle\langle\varphi_t| \quad \text{as } N \to \infty \tag{26}$$

where φ_t is the solution to the time-dependent Gross-Pitaevskii equation

$$i\partial_t \varphi_t = -\Delta\varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t \tag{27}$$

with initial data $\varphi_{t=0} = \varphi$.

The convergence in (25) and (26) is in the trace norm topology (which in this case is equivalent to the weak* topology defined on the space of trace class operators on $\mathbb{R}^3$). Moreover, from (26) we also get convergence of higher marginal. For every $k \geq 1$, we have

$$\gamma_{N,t}^{(k)} \to |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \quad \text{as } N \to \infty.$$

Theorem 1 can be used to describe the dynamics of condensates satisfying the condition of asymptotic factorization. The following two corollaries provide examples of such initial data.

The simplest example of N-particle wave function satisfying the assumption of asymptotic factorization is given by a product state.

Corollary 2. *Under the assumptions on $V(x)$ stated in Theorem 1, let $\psi_N(\mathbf{x}) = \prod_{j=1}^N \varphi(x_j)$ for an arbitrary $\varphi \in H^1(\mathbb{R}^3)$. Then, for any $t \in \mathbb{R}$,*

$$\gamma_{N,t}^{(1)} \to |\varphi_t\rangle\langle\varphi_t| \quad \text{as } N \to \infty$$

where φ_t is a solution of the Gross-Pitaevskii equation (27) with initial data $\varphi_{t=0} = \varphi$.

The second application of Theorem 1 gives a mathematical description of the results of the experiments depicted in the introduction.

Let

$$H_N^{\text{trap}} = \sum_{j=1}^{N} (-\Delta_j + V_{\text{ext}}(x_j)) + \sum_{i<j}^{N} V_N(x_i - x_j) \tag{28}$$

with a confining potential V_{ext}. Let ψ_N be the ground state of H_N^{trap}. By [9], ψ_N exhibits complete Bose Einstein condensation into the minimizer ϕ_{GP} of the Gross-Pitaevskii energy functional $\mathcal{E}_{\text{GP}}$ defined in (2). In other words

$$\gamma_N^{(1)} \to |\phi_{\text{GP}}\rangle\langle\phi_{\text{GP}}| \quad \text{as } N \to \infty.$$

In [7], we demonstrate that ψ_N also satisfies the condition (24) of asymptotic factorization. From this observation, we obtain the following corollary.

Corollary 3. *Under the assumptions on $V(x)$ stated in Theorem 1, let ψ_N be the ground state of (28), and denote by $\gamma_{N,t}^{(1)}$ the one-particle density associated with the solution $\psi_{N,t} = e^{-iH_N t}\psi_N$ of the Schrödinger equation (10). Then, for any fixed $t \in \mathbb{R}$,*

$$\gamma_{N,t}^{(1)} \to |\varphi_t\rangle\langle\varphi_t| \qquad \text{as } N \to \infty$$

where φ_t is the solution of the Gross-Pitaevskii equation (27) with initial data $\varphi_{t=0} = \phi_{GP}$.

Although the second corollary describes physically more realistic situations, also the first corollary has interesting consequences. In Sect. 2, we observed that the emergence of the scattering length in the Gross-Pitaevskii equation is an effect due to the correlations. The fact that the Gross-Pitaevskii equation describes the dynamics of the condensate also if the initial wave function is completely uncorrelated, as in Corollary 2, implies that the N-body Schrödinger dynamics generates the singular correlation structure in very short times. Of course, when the wave function develops correlations on the length scale $1/N$, the energy associated with this length scale decreases; since the total energy is conserved by the Schrödinger evolution, we must conclude that together with the short scale structure at scales of order $1/N$, the N-body dynamics also produces oscillations on intermediate length scales $1/N \ll \ell \ll 1$, which carry the excess energy (the difference between the energy of the factorized wave function and the energy of the wave function with correlations on the length scale $1/N$) and which have no effect on the macroscopic dynamics (because only variations of the wave function on length scales of order one and order $1/N$ affect the macroscopic dynamics described by the Gross-Pitaevskii equation).

4 General Strategy of the Proof and Previous Results

In this section we illustrate the strategy used to prove Theorem 1. The proof is divided into three main steps.

Step 1. Compactness of $\gamma_{N,t}^{(k)}$. Recall, from (11), the definition of the marginal densities $\gamma_{N,t}^{(k)}$ associated with the solution $\psi_{N,t} = \exp(-iH_N t)\psi_N$ of the N-body Schrödinger equation. By definition, for any $N \in \mathbb{N}$ and $t \in \mathbb{R}$, $\gamma_{N,t}^{(k)}$ is a positive operator in $\mathscr{L}_k^1 = \mathscr{L}^1(L^2(\mathbb{R}^{3k}))$ (the space of trace class operators on $L^2(\mathbb{R}^{3k})$) with trace equal to one. For fixed $t \in \mathbb{R}$ and $k \geq 1$, it follows by standard general argument (Banach-Alaouglu Theorem) that the sequence $\{\gamma_{N,t}^{(k)}\}_{N\geq k}$ is compact with respect to the weak* topology of $\mathscr{L}_k^1$. Note here that $\mathscr{L}_k^1$ has a weak* topology because $\mathscr{L}_k^1 = \mathscr{K}_k^*$, where $\mathscr{K}_k = \mathscr{K}(L^2(\mathbb{R}^{3k}))$ is the space of compact operators on $L^2(\mathbb{R}^{3k})$. To make sure that we can find subsequences of $\gamma_{N,t}^{(k)}$ which converge for all times in a certain interval, we fix $T > 0$ and consider the space $C([0,T], \mathscr{L}_k^1)$ of all functions of $t \in [0,T]$ with values in $\mathscr{L}_k^1$ which are continuous with respect to the weak* topology on $\mathscr{L}_k^1$. Since $\mathscr{K}_k$ is separable, it follows that the weak* topology on the unit ball of $\mathscr{L}_k^1$ is metrizable; this allows us to prove the equicontinuity of the densities $\gamma_{N,t}^{(k)}$, and to obtain compactness of the sequences $\{\gamma_{N,t}^{(k)}\}_{N\geq k}$ in $C([0,T], \mathscr{L}_k^1)$.

Step 2. Convergence to an infinite hierarchy. By Step 1 we know that, as $N \to \infty$, the family of marginal densities $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k=1}^N$ has at least one limit point $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k\geq 1}$ in $\bigoplus_{k\geq 1} C([0,T], \mathscr{L}_k^1)$ with respect to the product topology. Next, we derive evolution equations for the limiting densities $\gamma_{\infty,t}^{(k)}$. Starting from the BBGKY hierarchy (14) for the family $\Gamma_{N,t}$, we prove that any limit point $\Gamma_{\infty,t}$ satisfies the infinite hierarchy of equations

$$i\partial_t \gamma_{\infty,t}^{(k)} = \sum_{j=1}^k \left[-\Delta_j, \gamma_{\infty,t}^{(k)}\right] + 8\pi a_0 \sum_{j=1}^k \mathrm{Tr}_{k+1}\left[\delta(x_j - x_{k+1}), \gamma_{\infty,t}^{(k+1)}\right] \tag{29}$$

for $k \geq 1$. It is at this point, in the derivation of this infinite hierarchy, that we need to identify the singular part of the densities $\gamma_{N,t}^{(k+1)}$. The emergence of the scattering length in the second term on the right hand side of (29) is due to short scale structure of $\gamma_{N,t}^{(k+1)}$.

It is worth noticing that the infinite hierarchy (29) has a factorized solution. In fact, it is simple to see that the infinite family

$$\gamma_t^{(k)} = |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \quad \text{for } k \geq 1 \tag{30}$$

solves (29) if and only if φ_t is a solution to the Gross-Pitaevskii equation (27).

Step 3. Uniqueness of the solution to the infinite hierarchy. To conclude the proof of Theorem 1, we show that the infinite hierarchy (29) has a unique solution. This

implies immediately that the densities $\gamma^{(k)}_{N,t}$ converge; in fact, a compact sequence with at most one limit point is always convergent. Moreover, since we know that the factorized densities (30) are a solution, it also follows that, for any $k \geq 1$,

$$\gamma^{(k)}_{N,t} \to |\varphi_t\rangle\langle\varphi_t|^{\otimes k} \quad \text{as } N \to \infty$$

with respect to the weak* topology of $\mathscr{L}^1_k$.

Similar strategies have been used to obtain rigorous derivations of the nonlinear Hartree equation

$$i\partial_t \varphi_t = -\Delta\varphi_t + (v * |\varphi_t|^2)\varphi_t \tag{31}$$

for the dynamics of initially factorized wave functions in bosonic many particle mean field models, characterized by the Hamiltonian

$$H^{\mathrm{mf}}_N \sum_{j=1}^N -\Delta_j + \frac{1}{N}\sum_{i<j}^N v(x_i - x_j). \tag{32}$$

In this context, the approach outlined above was introduced by Spohn in [11], who applied it to derive (31) in the case of a bounded potential v. In [5], Erdős and Yau extended Spohn's result to the case of a Coulomb interaction $v(x) = \pm 1/|x|$ (partial results for the Coulomb case, in particular the convergence to the infinite hierarchy, were also obtained by Bardos, Golse, and Mauser, see [3]). More recently, Adami, Golse, and Teta used the same approach in [1] for one-dimensional systems with dynamics generated by a Hamiltonian of the form (32) with an N-dependent pair potential $v_N(x) = N^\beta V(N^\beta x)$, $\beta < 1$. In the limit $N \to \infty$, they obtain the nonlinear Schrödinger equation

$$i\partial_t\varphi_t = -\Delta\varphi_t + b_0|\varphi_t|^2\varphi_t \quad \text{with } b_0 = \int V(x)\mathrm{d}x.$$

Notice that the Hamiltonian (9) has the same form as the mean field Hamiltonian (32), with an N-dependent pair potential $v_N(x) = N^3 V(Nx)$. Of course, one may also ask what happens if we consider the mean field Hamiltonian (32) with the N-dependent potential $v_N(x) = N^{3\beta}V(N^\beta x)$, for $\beta \neq 1$. If $\beta < 1$, the short scale structure developed by the solution of the Schrödinger equation is still characterized by the length scale $1/N$ (because the scattering length of $N^{3\beta-1}V(N^\beta x)$ is still of order $1/N$); but this time the potential varies on much larger scales, of the order $N^{-\beta} \gg N^{-1}$. For this reason, if $\beta < 1$, the scattering length does not appear in the effective macroscopic equation ($8\pi a_0$ is replaced by $b_0 = \int \mathrm{d}x\, V(x)$). In [8] (and previously in [7] for $0 < \beta < 1/2$) we prove in fact that Corollary 2 can be extended to include the case $0 < \beta < 1$ as follows.

Theorem 4. *Suppose $\psi_N(\mathbf{x}) = \prod_{j=1}^N \varphi(x_j)$, for some $\varphi \in H^1(\mathbb{R}^3)$. Let $\psi_{N,t} = e^{-iH_{\beta,N}t}\psi_N$ with the mean-field Hamiltonian*

$$H_{\beta,N} = \sum_{j=1}^{N} -\Delta_j + \frac{1}{N} \sum_{i<j}^{N} N^{3\beta} V(N^\beta (x_i - x_j))$$

for a positive, spherical symmetric, compactly supported, and smooth potential V such that α (defined in (23)) is sufficiently small. Let $\gamma^{(1)}_{N,t}$ be the one-particle density associated with $\psi_{N,t}$. Then, if $0 < \beta \leq 1$ we have, for any fixed $t \in \mathbb{R}$, $\gamma^{(1)}_{N,t} \to |\varphi_t\rangle\langle\varphi_t|$ as $N \to \infty$. Here φ_t is the solution to the nonlinear Schrödinger equation

$$i\,\partial_t \varphi_t = -\Delta \varphi_t + \sigma |\varphi_t|^2 \varphi_t$$

with initial data $\varphi_{t=0} = \varphi$ and with

$$\sigma = \begin{cases} 8\pi a_0 & \text{if } \beta = 1, \\ b_0 & \text{if } 0 < \beta < 1. \end{cases}$$

5 Convergence to the Infinite Hierarchy

In this section we give some more details concerning Step 2 in the strategy outlined above. We consider a limit point $\Gamma_{\infty,t} = \{\gamma^{(k)}_{\infty,t}\}_{k\geq 1}$ of the sequence $\Gamma_{N,t} = \{\gamma^{(k)}_{N,t}\}_{k=1}^{N}$ and we prove that $\Gamma_{\infty,t}$ satisfies the infinite hierarchy (29). To this end we use that, for finite N, the family $\Gamma_{N,t}$ satisfies the BBGKY hierarchy (14), and we show the convergence of each term in (14) to the corresponding term in the infinite hierarchy (29) (the second term on the r.h.s. of (14) is of smaller order and can be proven to vanish in the limit $N \to \infty$).

The main difficulty consists in proving the convergence of the last term on the right hand side of (14) to the last term on the right hand side of (29). In particular, we need to show that in the limit $N \to \infty$ we can replace the potential $(N-k)N^2 V(N(x_j - x_{k+1})) \simeq N^3 V(Nx)$ in the last term on the r.h.s. of (14) by $8\pi a_0 \delta(x_j - x_{k+1})$. In terms of kernels we have to prove that

$$\int \mathrm{d}x_{k+1} (N^3 V(N(x_j - x_{k+1})) - 8\pi a_0 \delta(x_j - x_{k+1})) \gamma^{(k+1)}_{N,t}(\mathbf{x}_k, x_{k+1}, \mathbf{x}'_k, x_{k+1}) \to 0 \tag{33}$$

as $N \to \infty$. It is enough to prove the convergence (33) in a weak sense, after testing the expression against a smooth k-particle kernel $J^{(k)}(\mathbf{x}_k; \mathbf{x}'_k)$. Note, however, that the observable $J^{(k)}$ does not help to perform the integration over the variable x_{k+1}.

The problem here is that, formally, the N-dependent potential $N^3 V(N(x_j - x_{k+1}))$ does not converge towards $8\pi a_0 \delta(x_j - x_{k+1})$ as $N \to \infty$ (it converges towards $b_0 \delta(x_j - x_{k+1})$, with $b_0 = \int \mathrm{d}x\, V(x)$). Equation (33) is only correct because of the correlations between x_j and x_{k+1} hidden in the density $\gamma^{(k+1)}_{N,t}$. Therefore, to prove (33), we start by factoring out the correlations explicitly, and by proving that, as $N \to \infty$,

$$\int \mathrm{d}x_{k+1} \big(N^3 V(N(x_j - x_{k+1})) f_N(x_j - x_{k+1}) - 8\pi a_0 \delta(x_j - x_{k+1}) \big) \frac{\gamma_{N,t}^{(k+1)}(\mathbf{x}_k, x_{k+1}, \mathbf{x}'_k, x_{k+1})}{f_N(x_j - x_{k+1})} \to 0 \tag{34}$$

where $f_N(x)$ is the solution to the zero energy scattering equation (8). Then, in a second step, we use the fact that $f_N \to 1$ in the weak limit $N \to \infty$, to prove that the ratio $\gamma_{N,t}^{(k+1)}/f_N(x_j - x_{k+1})$ converges to the same limiting density $\gamma_{\infty,t}^{(k+1)}$ as $\gamma_{N,t}^{(k+1)}$. Equation (34) looks now much better than (33) because, formally, $N^3 V(N(x_j - x_{k+1})) f_N(x_j - x_{k+1})$ does converge to $8\pi a_0 \delta(x_j - x_{k+1})$. To prove that (34) is indeed correct, we only need some regularity of the ratio $\gamma_{N,t}^{(k+1)}(\mathbf{x}_k, x_{k+1}; \mathbf{x}'_k, x_{k+1})/f_N(x_j - x_{k+1})$ in the variables x_j and x_{k+1}. In terms of the N-particle wave function $\psi_{N,t}$ we need regularity of $\psi_{N,t}(\mathbf{x})/f_N(x_i - x_j)$ in the variables x_i, x_j, for any $i \neq j$. To establish the required regularity we use the following energy estimate.

Proposition 5. *Consider the Hamiltonian H_N defined in (9), with a positive, spherical symmetric, smooth and compactly supported potential V. Suppose that α (defined in (23)) is sufficiently small. Then there exists $C = C(\alpha) > 0$ such that*

$$\langle \psi, H_N^2 \psi \rangle \geq C N^2 \int \mathrm{d}\mathbf{x} \left| \nabla_i \nabla_j \frac{\psi(\mathbf{x})}{f_N(x_i - x_j)} \right|^2 \tag{35}$$

for all $i \neq j$ and for all $\psi \in L^2_s(\mathbb{R}^{3N}, \mathrm{d}\mathbf{x})$.

Making use of this energy estimate it is possible to deduce strong a-priori bounds on the solution $\psi_{N,t}$ of the Schrödinger equation (10). These bounds have the form

$$\int \mathrm{d}\mathbf{x} \left| \nabla_i \nabla_j \frac{\psi_{N,t}(\mathbf{x})}{f_N(x_i - x_j)} \right|^2 \leq C \tag{36}$$

uniformly in $N \in \mathbb{N}$ and $t \in \mathbb{R}$. To prove (36) we use that, by (35), and because of the conservation of the energy along the time evolution,

$$\begin{aligned} \int \mathrm{d}\mathbf{x} \left| \nabla_i \nabla_j \frac{\psi_{N,t}(\mathbf{x})}{f_N(x_i - x_j)} \right|^2 &\leq C N^{-2} \langle \psi_{N,t}, H_N^2 \psi_{N,t} \rangle \\ &= C N^{-2} \langle \psi_{N,0}, H_N^2 \psi_{N,0} \rangle. \end{aligned} \tag{37}$$

From (37) and using an approximation argument on the initial wave function to make sure that the expectation of H_N^2 at time $t = 0$ is of the order N^2, we obtain (36).

The bounds (36) are then sufficient to prove the convergence (33) (using a non-standard Poincaré inequality; see Lemma 7.2 in [8]).

Remark that the a-priori bounds (36) do not hold true if we do not divide the solution $\psi_{N,t}$ of the Schrödinger equation by $f_N(x_i - x_j)$ (replacing $\psi_{N,t}(\mathbf{x})/f_N(x_i - x_j)$ by $\psi_N(\mathbf{x})$ the integral in (36) would be of order N). It is only after removing the

singular factor $f_N(x_i - x_j)$ from $\psi_{N,t}(\mathbf{x})$ that we can prove useful bounds on the regular part of the wave function.

It is through the a-priori bounds (36) that we identify the correlation structure of the wave function $\psi_{N,t}$ and that we show that, when x_i and x_j are close to each other, $\psi_{N,t}(\mathbf{x})$ can be approximated by the time independent singular factor $f_N(x_i - x_j)$, which varies on the length scale $1/N$, multiplied with a regular part (regular in the sense that it satisfy the bounds (36)). It is therefore through (36) that we establish the strong separation of scales in the wave function $\psi_{N,t}$ and in the marginal densities $\gamma^{(k)}_{N,t}$ which is of fundamental importance for the Gross-Pitaevskii theory.

Since it is quite short and it shows why the solution $f_N(x_i - x_j)$ to the zero energy scattering equation (5) can be used to describe the two-particle correlations, we reproduce in the following the proof of Proposition 5. Note that this is the only step in the proof of our main theorem where the smallness of the constant α, measuring the strength of the interaction potential, is used. The positivity of the interaction potential, on the other hand, also plays an important role in many other parts of the proof.

Proof (of Proposition 5). We decompose the Hamiltonian (9) as

$$H_N = \sum_{j=1}^N h_j \qquad \text{with} \qquad h_j = -\Delta_j + \frac{1}{2}\sum_{i\neq j} V_N(x_i - x_j).$$

For an arbitrary permutation symmetric wave function ψ and for any fixed $i \neq j$, we have

$$\langle \psi, H_N^2 \psi\rangle = N\langle \psi, h_i^2 \psi\rangle + N(N-1)\langle \psi, h_i h_j \psi\rangle \geq N(N-1)\langle \psi, h_i h_j \psi\rangle.$$

Using the positivity of the potential, we find

$$\begin{aligned}&\langle \psi, H_N^2 \psi\rangle \\ &\quad \geq N(N-1)\left\langle \psi, \left(-\Delta_i + \frac{1}{2}V_N(x_i - x_j)\right)\left(-\Delta_j + \frac{1}{2}V_N(x_i - x_j)\right)\psi\right\rangle. \end{aligned} \tag{38}$$

Next, we define $\phi(\mathbf{x})$ by $\psi(\mathbf{x}) = f_N(x_i - x_j)\phi(\mathbf{x})$ (ϕ is well defined because $f_N(x) > 0$ for all $x \in \mathbb{R}^3$); note that the definition of the function ϕ depends on the choice of i, j. Then

$$\begin{aligned}&\frac{1}{f_N(x_i - x_j)}\Delta_i(f_N(x_i - x_j)\phi(\mathbf{x})) \\ &\quad = \Delta_i\phi(\mathbf{x}) + \frac{(\Delta f_N)(x_i - x_j)}{f_N(x_i - x_j)}\phi(\mathbf{x}) + \frac{\nabla f_N(x_i - x_j)}{f_N(x_i - x_j)}\nabla_i\phi(\mathbf{x}). \end{aligned} \tag{39}$$

From (5) it follows that

$$\frac{1}{f_N(x_i - x_j)}\left(-\Delta_i + \frac{1}{2}V_N(x_i - x_j)\right)f_N(x_i - x_j)\phi(\mathbf{x}) = L_i\phi(\mathbf{x})$$

and analogously

$$\frac{1}{f_N(x_i - x_j)}\left(-\Delta_j + \frac{1}{2}V_N(x_i - x_j)\right) f_N(x_i - x_j)\phi(\mathbf{x}) = L_j\phi(\mathbf{x})$$

where we defined

$$L_\ell = -\Delta_\ell + 2\frac{\nabla_\ell f_N(x_i - x_j)}{f_N(x_i - x_j)}\nabla_\ell, \quad \text{for } \ell = i, j.$$

Remark that, for $\ell = i, j$, the operator L_ℓ satisfies

$$\begin{aligned}\int \mathrm{d}\mathbf{x} f_N^2(x_i - x_j) L_\ell \overline{\phi}(\mathbf{x})\psi(\mathbf{x}) &= \int \mathrm{d}\mathbf{x} f_N^2(x_i - x_j)\overline{\phi}(\mathbf{x}) L_\ell\psi(\mathbf{x}) \\ &= \int \mathrm{d}\mathbf{x} f_N^2(x_i - x_j)\nabla_\ell\overline{\phi}(\mathbf{x})\nabla_\ell\psi(\mathbf{x}). \end{aligned} \tag{40}$$

Therefore, from (38), we obtain

$$\begin{aligned}\langle\psi, H_N^2\psi\rangle &\geq N(N-1)\int \mathrm{d}\mathbf{x} f_N^2(x_i - x_j) L_i\overline{\phi}(\mathbf{x}) L_j\phi(\mathbf{x}) \\ &= N(N-1)\int \mathrm{d}\mathbf{x} f_N^2(x_i - x_j)\nabla_i\overline{\phi}(\mathbf{x})\nabla_i L_j\phi(\mathbf{x}) \\ &= N(N-1)\int \mathrm{d}\mathbf{x} f_N^2(x_i - x_j)\nabla_i\overline{\phi}(\mathbf{x}) L_j\nabla_i\phi(\mathbf{x}) \\ &\quad + N(N-1)\int \mathrm{d}\mathbf{x} f_N^2(x_i - x_j)\nabla_i\overline{\phi}(\mathbf{x})[\nabla_i, L_j]\phi(\mathbf{x}) \\ &= N(N-1)\int \mathrm{d}\mathbf{x} f_N^2(x_i - x_j)|\nabla_j\nabla_i\phi(\mathbf{x})|^2 \\ &\quad + N(N-1)\int \mathrm{d}\mathbf{x} f_N^2(x_i - x_j)\left(\nabla_i\frac{\nabla f_N(x_i - x_j)}{f_N(x_i - x_j)}\right)\nabla_i\overline{\phi}(\mathbf{x})\nabla_j\phi(\mathbf{x}). \end{aligned} \tag{41}$$

To control the second term on the right hand side of the last equation we use bounds on the function f_N, which can be derived from the zero energy scattering equation (5):

$$1 - C\alpha \leq f_N(x) \leq 1, \quad |\nabla f_N(x)| \leq C\frac{\alpha}{|x|}, \quad |\nabla^2 f_N(x)| \leq C\frac{\alpha}{|x|^2} \tag{42}$$

for constants C independent of N and of the potential V (recall the definition of the dimensionless constant α from (23)). Therefore, for $\alpha < 1$,

$$\begin{aligned}\left| \int \mathrm{d}\mathbf{x} f_N^2(x_i - x_j) \left(\nabla_i \frac{\nabla f_N(x_i - x_j)}{f_N(x_i - x_j)} \right) \nabla_i \overline{\phi}(\mathbf{x}) \nabla_j \phi(\mathbf{x}) \right| \\ \leq C\alpha \int \mathrm{d}\mathbf{x} \frac{1}{|x_i - x_j|^2} |\nabla_i \phi(\mathbf{x})| |\nabla_j \phi(\mathbf{x})| \\ \leq C\alpha \int \mathrm{d}\mathbf{x} \frac{1}{|x_i - x_j|^2} \left(|\nabla_i \phi(\mathbf{x})|^2 + |\nabla_j \phi(\mathbf{x})|^2 \right) \\ \leq C\alpha \int \mathrm{d}\mathbf{x} |\nabla_i \nabla_j \phi(\mathbf{x})|^2 \end{aligned} \tag{43}$$

where we used Hardy inequality. Thus, from (41), and using again the first bound in (42), we obtain

$$\langle \psi, H_N^2 \psi \rangle \geq N(N-1)(1 - C\alpha) \int \mathrm{d}\mathbf{x} |\nabla_i \nabla_j \phi(\mathbf{x})|^2$$

which implies (35). □

6 Uniqueness of the Solution to the Infinite Hierarchy

In this section we discuss the main ideas used to prove the uniqueness of the solution to the infinite hierarchy (Step 3 in the strategy outlined in Sect. 4).

First of all, we need to specify in which class of family of densities $\Gamma_t = \{\gamma_t^{(k)}\}_{k \geq 1}$ we want to prove the uniqueness of the solution to the infinite hierarchy (29). Clearly, the proof of the uniqueness is simpler if we can restrict our attention to smaller classes. But of course, in order to apply the uniqueness result to prove Theorem 1, we need to make sure that any limit point of the sequence $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k=1}^N$ is in the class for which we can prove uniqueness.

We are going to prove uniqueness for all families $\Gamma_t = \{\gamma_t^{(k)}\}_{k \geq 1} \in \oplus C([0,T], \mathscr{L}_k^1)$ with

$$\begin{aligned}\|\gamma_t^{(k)}\|_{\mathscr{H}_k} &:= \mathrm{Tr} |(1 - \Delta_1)^{1/2} \dots (1 - \Delta_k)^{1/2} \gamma_t^{(k)} (1 - \Delta_k)^{1/2} \dots (1 - \Delta_1)^{1/2}| \\ &\leq C^k \end{aligned} \tag{44}$$

for all $t \in [0,T]$ and for all $k \geq 1$ (with a constant C independent of k).

The following proposition guarantees that any limit point of the sequence $\Gamma_{N,t}$ satisfies (44).

Proposition 6. *Assume the same conditions as in Proposition 5. Suppose that $\Gamma_{\infty,t} = \{\gamma_{\infty,t}^{(k)}\}_{k \geq 1}$ is a limit point of $\Gamma_{N,t} = \{\gamma_{N,t}^{(k)}\}_{k=1}^N$ with respect to the product topology on $\bigoplus_{k \geq 1} C([0,T], \mathscr{L}_k^1)$. Then $\gamma_{\infty,t}^{(k)} \geq 0$ and there exists a constant C such that*

$$\mathrm{Tr}(1 - \Delta_1) \dots (1 - \Delta_k) \gamma_{\infty,t}^{(k)} \leq C^k \tag{45}$$

for all $k \geq 1$ and $t \in [0,T]$.

Because of Proposition 6, it is enough to prove the uniqueness of the infinite hierarchy (29) in the following sense.

Theorem 7. *Suppose that* $\Gamma = \{\gamma^{(k)}\}_{k\geq 1}$ *is such that*

$$\|\gamma^{(k)}\|_{\mathscr{H}_k^-} \leq C^k \tag{46}$$

for all $k \geq 1$ (*the norm* $\|.\|_{\mathscr{H}_k^-}$ *is defined in* (44)). *Then there exists at most one solution* $\Gamma_t = \{\gamma_t^{(k)}\}_{k\geq 1} \in \bigoplus C([0,T], \mathscr{L}_k)$ *of* (29) *such that* $\Gamma_{t=0} = \Gamma$ *and*

$$\|\gamma_t^{(k)}\|_{\mathscr{H}_k^-} \leq C^k \tag{47}$$

for all $k \geq 1$ *and all* $t \in [0,T]$ (*with the same constant* C *as in* (46)).

In the next two subsections we explain the main ideas of the proofs of Proposition 6 and Theorem 7.

6.1 Higher Order Energy Estimates

The main difficulty in proving Proposition 6 is the fact that the estimate (45) does not hold true if we replace $\gamma_{\infty,t}^{(k)}$ by the marginal density $\gamma_{N,t}^{(k)}$. More precisely,

$$\mathrm{Tr}(1-\Delta_1)\cdots(1-\Delta_k)\gamma_{N,t}^{(k)} \leq C^k \tag{48}$$

cannot hold true with a constant C independent of N. In fact, for finite N and $k > 1$, the k-particle density $\gamma_{N,t}^{(k)}$ still contains the short scale structure due to the correlations among the particles. Therefore, when we take derivatives of $\gamma_{N,t}^{(k)}$ as in (48), the singular structure (which varies on a length scale of order $1/N$) generates contributions which diverge in the limit $N \to \infty$.

To overcome this problem, we cutoff the wave function $\psi_{N,t}$ when two or more particles come at distances smaller than some intermediate length scale ℓ, with $N^{-1} \ll \ell \ll 1$ (more precisely, the cutoff will be effective only when one or more particles come close to one of the variable x_j over which we want to take derivatives). For fixed $j = 1, \ldots, N$, we define $\theta_j \in C^\infty(\mathbb{R}^{3N})$ such that

$$\theta_j(\mathbf{x}) \simeq \begin{cases} 1 & \text{if } |x_i - x_j| \gg \ell \text{ for all } i \neq j \\ 0 & \text{if there exists } i \neq j \text{ with } |x_i - x_j| \lesssim \ell \end{cases}.$$

It is important, for our analysis, that θ_j controls its derivatives (in the sense that, for example, $|\nabla_i \theta_j| \leq C\ell^{-1}\theta_j^{1/2}$); for this reason we cannot use standard compactly supported cutoffs, but instead we have to construct appropriate functions which decay exponentially when particles come close together. Making use of the functions $\theta_j(\mathbf{x})$, we prove the following higher order energy estimates.

Proposition 8. *Choose $\ell \ll 1$ such that $N\ell^2 \gg 1$. Suppose that α is small enough. Then there exist constants C_1 and C_2 such that, for any $\psi \in L^2_s(\mathbb{R}^{3N})$,*

$$\langle \psi, (H_N + C_1 N)^k \psi \rangle \geq C_2 N^k \int \mathrm{d}\mathbf{x} \theta_1(\mathbf{x}) \cdots \theta_{k-1}(\mathbf{x}) |\nabla_1 \cdots \nabla_k \psi(\mathbf{x})|^2. \tag{49}$$

The meaning of the bounds (49) is clear. We can control the L^2-norm of the k-th derivative $\nabla_1 \cdots \nabla_k \psi$ by the expectation of the k-th power of the energy per particle, if we only integrate over configurations where the first $k-1$ particles are "isolated" (in the sense that there is no particle at distances smaller than ℓ from $x_1, x_2, \ldots, x_{k-1}$). In this sense the energy estimate in Proposition 5 (which, compared with Proposition 8, is restricted to $k = 2$) is more precise than (49), because it identifies and controls the singularity of the wave function exactly in the region cutoff from the integral on the right side of (49). The point is that, while Proposition 5 is used to identify the two-particle correlations in the marginal densities $\gamma^{(k)}_{N,t}$ (which are essential for the emergence of the scattering length a_0 in the infinite hierarchy (29)), we only need Proposition 8 to establish properties of the limiting densities; this is why we can introduce cutoffs in (49), provided we can show their effect to vanish in the limit $N \to \infty$.

Note that we can allow one "free derivative"; in (49) we take the derivative over x_k although there is no cutoff $\theta_k(\mathbf{x})$. The reason is that the correlation structure becomes singular, in the L^2-sense, only when we differentiate it twice (if one uses the zero energy solution f_N introduced in (5) to describe the correlations, this can be seen by observing that $\nabla f_N(x) \simeq 1/|x|$, which is locally square integrable). Remark that the condition $N\ell^2 \gg 1$ is a consequence of the fact that, if ℓ is too small, the error due to the localization of the kinetic energy on distances of order ℓ cannot be controlled. The proof of Proposition 8 is based on induction over k; for details see Sect. 9 in [8].

From the estimates (49), using the preservation of the expectation of H_N^k along the time evolution and a regularization of the initial N-particle wave function ψ_N, we obtain the following bounds for the solution $\psi_{N,t} = e^{-iH_N t}\psi_N$ of the Schrödinger equation (10).

$$\int \mathrm{d}\mathbf{x} \theta_1(\mathbf{x}) \cdots \theta_{k-1}(\mathbf{x}) |\nabla_1 \cdots \nabla_k \psi_{N,t}(\mathbf{x})|^2 \leq C^k \tag{50}$$

uniformly in N and t, and for all $k \geq 1$. Translating these bounds in the language of the density matrix $\gamma_{N,t}$, we obtain

$$\mathrm{Tr} \theta_1 \cdots \theta_{k-1} \nabla_1 \cdots \nabla_k \gamma_{N,t} \nabla_1^* \cdots \nabla_k^* \leq C^k. \tag{51}$$

The idea now is to use the freedom in the choice of the cutoff length ℓ. If we fix the position of all particles but x_j, it is clear that the cutoff θ_j is effective in a volume at most of the order $N\ell^3$. If we choose now ℓ such that $N\ell^3 \to 0$ as $N \to \infty$ (which is of course compatible with the condition that $N\ell^2 \gg 1$), then we can expect that, in the limit of large N, the cutoff becomes negligible. This approach yields in fact

the desired results; starting from (51), and choosing ℓ such that $N\ell^3 \ll 1$, we can complete the proof of Proposition 6 (see Proposition 6.3 in [8] for more details).

6.2 Expansion in Feynman Graphs

To prove Theorem 7, we start by rewriting the infinite hierarchy (29) in the integral form

$$\begin{aligned}\gamma_t &= \mathscr{U}^{(k)}(t)\gamma_0 + 8i\pi a_0 \sum_{j=1}^{k} \int_0^t \mathrm{d}s\, \mathscr{U}^{(k)}(t-s)\mathrm{Tr}_{k+1}\big[\delta(x_j - x_{k+1}), \gamma_s^{(k+1)}\big] \\ &= \mathscr{U}^{(k)}(t)\gamma_0 + \int_0^t \mathrm{d}s\, \mathscr{U}^{(k)}(t-s)B^{(k)}\gamma_s^{(k+1)} \end{aligned} \tag{52}$$

where $\mathscr{U}^{(k)}(t)$ denotes the free evolution of k particles,

$$\mathscr{U}^{(k)}(t)\gamma^{(k)} = e^{it\sum_{j=1}^{k}\Delta_j}\gamma^{(k)}e^{-it\sum_{j=1}^{k}\Delta_j}$$

and the collision operator $B^{(k)}$ maps $(k+1)$-particle operators into k-particle operators according to

$$B^{(k)}\gamma^{(k+1)} = 8i\pi a_0 \sum_{j=1}^{k} \mathrm{Tr}_{k+1}\big[\delta(x_j - x_{k+1}), \gamma^{(k+1)}\big] \tag{53}$$

(recall that Tr_{k+1} denotes the partial trace over the $(k+1)$-th particle).

Iterating (52) n times we obtain the Duhamel type series

$$\gamma_t^{(k)} = \mathscr{U}^{(k)}(t)\gamma_0^{(k)} + \sum_{m=1}^{n-1} \xi_{m,t}^{(k)} + \eta_{n,t}^{(k)} \tag{54}$$

with

$$\begin{aligned}\xi_{m,t}^{(k)} &= \int_0^t \mathrm{d}s_1 \cdots \int_0^{s_{m-1}} \mathrm{d}s_m\, \mathscr{U}^{(k)}(t-s_1)B^{(k)}\mathscr{U}^{(k+1)}(s_1-s_2)B^{(k+1)} \\ &\quad \cdots B^{(k+m-1)}\mathscr{U}^{(k+m)}(s_m)\gamma_0^{(k+m)} \\ &= \sum_{j_1=1}^{k}\sum_{j_2=1}^{k+1}\cdots\sum_{j_m=1}^{k+m}\int_0^t \mathrm{d}s_1 \cdots \int_0^{s_{m-1}} \mathrm{d}s_m\, \mathscr{U}^{(k)}(t-s_1)\mathrm{Tr}_{k+1}\big[\delta(x_{j_1} - x_{k+1}), \\ &\quad \mathscr{U}^{(k+1)}(s_1-s_2)\mathrm{Tr}_{k+2}\big[\delta(x_{j_2} - x_{k+2}), \dots \\ &\quad \mathrm{Tr}_{k+m}\big[\delta(x_{j_m} - x_{k+m}), \mathscr{U}^{(k+m)}(s_m)\gamma_0^{(k+m)}\big]\dots\big]\big] \end{aligned} \tag{55}$$

and the error term

$$\eta_{n,t}^{(k)} = \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2 \cdots \int_0^{s_{n-1}} \mathrm{d}s_n \, \mathscr{U}^{(k)}(t-s_1) B^{(k)} \mathscr{U}^{(k+1)}(s_1-s_2) B^{(k+1)} \cdots B^{(k+n-1)} \gamma_{s_n}^{(k+m)}. \tag{56}$$

Note that the error term (56) has exactly the same form as the terms in (55), with the only difference that the last free evolution is replaced by the full evolution $\gamma_{s_n}^{(k+m)}$.

To prove the uniqueness of the infinite hierarchy, it is enough to prove that the error term (56) converges to zero as $n \to \infty$ (in some norm, or even only after testing it against a sufficiently large class of smooth observables). The main problem here is that the delta function in the collision operator $B^{(k)}$ cannot be controlled by the kinetic energy (in the sense that, in three dimensions, the operator inequality $\delta(x) \leq C(1-\Delta)$ does not hold true). For this reason, the a priori estimates $\|\gamma_t^{(k)}\|_{\mathscr{H}_k} \leq C^k$ are not sufficient to show that (56) converges to zero, as $n \to \infty$. Instead, we have to make use of the smoothing effects of the free evolutions $\mathscr{U}^{(k+j)}(s_j - s_{j+1})$ in (56) (in a similar way, Stricharzt estimates are used to prove the well-posedness of nonlinear Schrödinger equations). To this end, we rewrite each term in the series (54) as a sum of contributions associated with certain Feynman graphs, and then we prove the convergence of the Duhamel expansion by controlling each contribution separately.

The details of the diagrammatic expansion can be found in Sect. 9 of [7]. Here we only present the main ideas. We start by considering the term $\xi_{m,t}^{(k)}$ in (55). After multiplying it with a compact k-particle observable $J^{(k)}$ and taking the trace, we expand the result as

$$\mathrm{Tr} J^{(k)} \xi_{m,t}^{(k)} = \sum_{\Lambda \in \mathscr{F}_{m,k}} K_{\Lambda,t} \tag{57}$$

where $K_{\Lambda,t}$ is the contribution associated with the Feynman graph Λ. Here $\mathscr{F}_{m,k}$ denotes the set of all graphs consisting of $2k$ disjoint, paired, oriented, and rooted trees with m vertices. An example of a graph in $\mathscr{F}_{m,k}$ is drawn in Fig. 1. Each vertex has one of the two forms drawn in Fig. 1, with one "father"-edge on the left (closer to the root of the tree) and three "son"-edges on the right. One of the son edge is marked (the one drawn on the same level as the father edge; the other two son edges

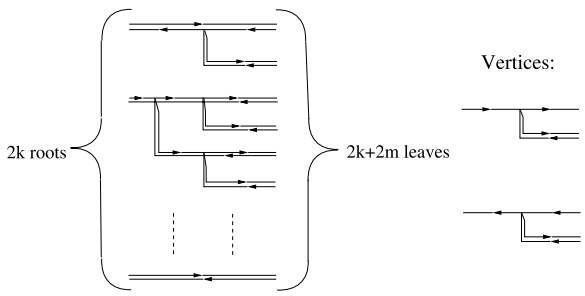

Fig. 1 A Feynman graph in $\mathscr{F}_{m,k}$ and its two types of vertices

are drawn below). Graphs in $\mathscr{F}_{m,k}$ have $2k+3m$ edges, $2k$ roots (the edges on the very left), and $2k+2m$ leaves (the edges on the very right). It is possible to show that the number of different graphs in $\mathscr{F}_{m,k}$ is bounded by 2^{4m+k}.

The particular form of the graphs in $\mathscr{F}_{m,k}$ is due to the quantum mechanical nature of the expansion; the presence of a commutator in the collision operator (53) implies that, for every $B^{(k+j)}$ in (55), we can choose whether to write the interaction on the left or on the right of the density. When we draw the corresponding vertex in a graph in $\mathscr{F}_{m,k}$, we have to choose whether to attach it on the incoming or on the outgoing edge.

Graphs in $\mathscr{F}_{m,k}$ are characterized by a natural partial ordering among the vertices ($v \prec v'$ if the vertex v is on the path from v' to the roots); there is, however, no total ordering. The absence of total ordering among the vertices is the consequence of a rearrangement of the summands on the r.h.s. of (55); by removing the order between times associated with non-ordered vertices we significantly reduce the number of terms in the expansion. In fact, while (55) contains $(m+k)!/k!$ summands, in (57) we are only summing over 2^{4m+k} contributions. The price we have to pay is that the apparent gain of a factor $1/m!$ because of the ordering of the time integrals in (55) is lost in the new expansion (57). However, since the time integrations are already needed to smooth out singularities, and since they cannot be used simultaneously for smoothing and for gaining a factor $1/m!$, it seems very difficult to make use of the apparent factor $1/m!$ in (55). In fact, we find that the expansion (57) is better suited for analyzing the cumulative space-time smoothing effects of the multiple free evolutions than (55).

Because of the pairing of the $2k$ trees, there is a natural pairing between the $2k$ roots of the graph. Moreover, it is also possible to define a natural pairing of the leaves of the graph (this is evident in Fig. 1); two leaves ℓ_1 and ℓ_2 are paired if there exists an edge e_1 on the path from ℓ_1 back to the roots, and an edge e_2 on the path from ℓ_2 to the roots, such that e_1 and e_2 are the two unmarked son-edges of the same vertex (or, if there is no unmarked sons in the path from ℓ_1 and ℓ_2 to the roots, if the two roots connected to ℓ_1 and ℓ_2 are paired).

For $\Lambda \in \mathscr{F}_{m,k}$, we denote by $E(\Lambda)$, $V(\Lambda)$, $R(\Lambda)$ and $L(\Lambda)$ the set of all edges, vertices, roots and, respectively, leaves in the graph Λ. For every edge $e \in E(\Lambda)$, we introduce a three-dimensional momentum variable p_e and a one-dimensional frequency variable α_e. Then, denoting by $\widehat{\gamma}_0^{(k+m)}$ and by $\widehat{J}^{(k)}$ the kernels of the density $\gamma_0^{(k+m)}$ and of the observable $J^{(k)}$ in Fourier space, the contribution $K_{\Lambda,t}$ in (57) is given by

$$\begin{aligned} K_{\Lambda,t} = \int \prod_{e\in E(\Lambda)} \frac{\mathrm{d}p_e \mathrm{d}\alpha_e}{\alpha_e - p_e^2 + i\tau_e\mu_e} \prod_{v\in V(\Lambda)} \delta\Big(\sum_{e\in v} \pm\alpha_e\Big)\delta\Big(\sum_{e\in v} \pm p_e\Big) \\ \times \exp\Big(-it \sum_{e\in R(\Lambda)} \tau_e(\alpha_e + i\tau_e\mu_e)\Big) \widehat{J}^{(k)}(\{p_e\}_{e\in R(\Lambda)}) \\ \times \widehat{\gamma}_0^{(k+m)}(\{p_e\}_{e\in L(\Lambda)}). \end{aligned} \tag{58}$$

Here $\tau_e = \pm 1$, according to the orientation of the edge e. We observe from (58) that the momenta of the roots of Λ are the variables of the kernel of $J^{(k)}$, while the momenta of the leaves of Λ are the variables of the kernel of $\gamma_0^{(k+m)}$ (this also explain why roots and leaves of Λ need to be paired).

The denominators $(\alpha_e - p_e^2 + i\tau_e\mu_e)^{-1}$ are called propagators; they correspond to the free evolutions in the expansion (55) and they enter the expression (58) through the formula

$$e^{itp^2} = \int_{-\infty}^{\infty} \mathrm{d}\alpha \, \frac{e^{it(\alpha+i\mu)}}{\alpha - p^2 + i\mu}$$

(here and in (58) the measure $\mathrm{d}\alpha$ is defined by $\mathrm{d}\alpha = \mathrm{d}'\alpha/(2\pi i)$ where $\mathrm{d}'\alpha$ is the Lebesgue measure on $\mathbb{R}$).

The regularization factors μ_e in (58) have to be chosen such that $\mu_{\text{father}} = \sum_{e=\text{ son}} \mu_e$ at every vertex. The delta-functions in (58) express momentum and frequency conservation (the sum over $e \in v$ denotes the sum over all edges adjacent to the vertex v; here $\pm\alpha_e = \alpha_e$ if the edge points towards the vertex, while $\pm\alpha_e = -\alpha_e$ if the edge points out of the vertex, and analogously for $\pm p_e$).

An analogous expansion can be obtained for the error term $\eta_{n,t}^{(k)}$ in (56). The problem now is to analyze the integral (58) (and the corresponding integral for the error term). Through an appropriate choice of the regularization factors μ_e one can extract the time dependence of $K_{\Lambda,t}$ and show that

$$\begin{aligned} |K_{\Lambda,t}| \leq C^{k+m} t^{m/4} \int \prod_{e\in E(\Gamma)} \frac{\mathrm{d}\alpha_e \mathrm{d}p_e}{\langle \alpha_e - p_e^2 \rangle} \prod_{v\in V(\Gamma)} \delta\Big(\sum_{e\in v} \pm\alpha_e\Big) \delta\Big(\sum_{e\in v} \pm p_e\Big) \\ \times \big|\widehat{J}^{(k)}(\{p_e\}_{e\in R(\Gamma)})\big| \big|\widehat{\gamma}_0^{(k+m)}(\{p_e\}_{e\in L(\Gamma)})\big| \end{aligned} \tag{59}$$

where we introduced the notation $\langle x \rangle = (1+x^2)^{1/2}$.

Because of the singularity of the interaction at zero, we may be faced here with an ultraviolet problem; we have to show that all integrations in (59) are finite in the regime of large momenta and large frequency. Because of (46), we know that the kernel $\widehat{\gamma}_0^{(k+m)}(\{p_e\}_{e\in L(\Lambda)})$ in (59) provides decay in the momenta of the leaves. From (46) we have, in momentum space,

$$\int \mathrm{d}p_1 \cdots \mathrm{d}p_n (p_1^2+1)\cdots(p_n^2+1) \widehat{\gamma}_0^{(n)}(p_1,\ldots,p_n;p_1,\ldots,p_n) \leq C^n$$

for all $n \geq 1$. Power counting implies that

$$|\widehat{\gamma}_0^{(k+m)}(\{p_e\}_{e\in L(\Lambda)})| \lesssim \prod_{e\in L(\Lambda)} \langle p_e \rangle^{-5/2}. \tag{60}$$

Using this decay in the momenta of the leaves and the decay of the propagators $\langle \alpha_e - p_e^2 \rangle^{-1}$, $e \in E(\Lambda)$, we can prove the finiteness of all the momentum and frequency integrals in (58). Heuristically, this can be seen using a simple power

counting argument. Fix $\kappa \gg 1$, and cutoff all momenta $|p_e| \geq \kappa$ and all frequencies $|\alpha_e| \geq \kappa^2$. Each p_e-integral scales then as κ^3, and each α_e-integral scales as κ^2. Since we have $2k + 3m$ edges in Λ, we have $2k + 3m$ momentum- and frequency integrations. However, because of the m delta functions (due to momentum and frequency conservation), we effectively only have to perform $2k + 2m$ momentum- and frequency-integrations. Therefore the whole integral in (58) carries a volume factor of the order $\kappa^{5(2k+2m)} = \kappa^{10k+10m}$. Now, since there are $2k + 2m$ leaves in the graph Λ, the estimate (60) guarantees a decay of the order $\kappa^{-5/2(2k+2m)} = \kappa^{-5k-5m}$. The $2k + 3m$ propagators, on the other hand, provide a decay of the order $\kappa^{-2(2k+3m)} = \kappa^{-4k-6m}$. Choosing the observable $J^{(k)}$ so that $\widehat{J}^{(k)}$ decays sufficiently fast at infinity, we can also gain an additional decay κ^{-6k}. Since

$$\kappa^{10k+10m} \cdot \kappa^{-5k-5m-4k-6m-6k} = \kappa^{-m-5k} \ll 1$$

for $\kappa \gg 1$, we can expect (58) to converge in the large momentum and large frequency regime. Remark the importance of the decay provided by the free evolution (through the propagators); without making use of it, we would not be able to prove the uniqueness of the infinite hierarchy.

This heuristic argument is clearly far from rigorous. To obtain a rigorous proof, we use an integration scheme dictated by the structure of the graph Λ; we start by integrating the momenta and the frequency of the leaves (for which (60) provides sufficient decay). The point here is that when we perform the integrations over the momenta of the leaves we have to propagate the decay to the next edges on the left. We move iteratively from the right to the left of the graph, until we reach the roots; at every step we integrate the frequencies and momenta of the son edges of a fixed vertex and as a result we obtain decay in the momentum of the father edge. When we reach the roots, we use the decay of the kernel $\widehat{J}^{(k)}$ to complete the integration scheme. In a typical step, we consider a vertex as the one drawn in Fig. 2 and we assume to have decay in the momenta of the three son-edges, in the form $|p_e|^{-\lambda}$, $e = u, d, w$ (for some $2 < \lambda < 5/2$). Then we integrate over the frequencies $\alpha_u, \alpha_d, \alpha_w$ and the momenta p_u, p_d, p_w of the son-edges and as a result we obtain a decaying factor $|p_r|^{-\lambda}$ in the momentum of the father edge. In other words, we prove bounds of the form

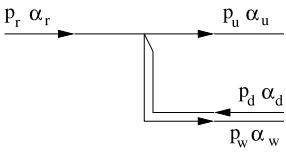

Fig. 2 Integration scheme: a typical vertex

$$\int \frac{\mathrm{d}\alpha_u \mathrm{d}\alpha_d \mathrm{d}\alpha_w \mathrm{d}p_u \mathrm{d}p_d \mathrm{d}p_w}{|p_u|^\lambda |p_d|^\lambda |p_w|^\lambda} \frac{\delta(\alpha_r = \alpha_u + \alpha_d - \alpha_w)\delta(p_r = p_u + p_d - p_w)}{\langle \alpha_u - p_u^2\rangle \langle \alpha_d - p_d^2\rangle \langle \alpha_w - p_w^2\rangle} \leq \frac{\text{const}}{|p_r|^\lambda}. \tag{61}$$

Power counting implies that (61) can only be correct if $\lambda > 2$. On the other hand, to start the integration scheme we need $\lambda < 5/2$ (from (60) this is the decay in the momenta of the leaves, obtained from the a-priori estimates). It turns out that, choosing $\lambda = 2 + \varepsilon$ for a sufficiently small $\varepsilon > 0$, (61) can be made precise, and the integration scheme can be completed.

After integrating all the frequency and momentum variables, from (59) we obtain that

$$|K_{\Lambda,t}| \leq C^{k+m} t^{m/4}$$

for every $\Lambda \in \mathscr{F}_{m,k}$. Since the number of diagrams in $\mathscr{F}_{m,k}$ is bounded by C^{k+m}, it follows immediately that

$$\left|\mathrm{Tr} J^{(k)} \xi^{(k)}_{m,t}\right| \leq C^{k+m} t^{m/4}.$$

Note that, from (55), one may expect $\xi^{(k)}_{m,t}$ to be proportional to t^m. The reason why we only get a bound proportional to $t^{m/4}$ is that we effectively use part of the time integration to control the singularity of the potentials.

Note that the only property of $\gamma_0^{(k+m)}$ used in the analysis of (58) is the estimate (46), which provides the necessary decay in the momenta of the leaves. However, since the a-priori bound (47) hold uniformly in time, we can use a similar argument to bound the contribution arising from the error term $\eta^{(k)}_{n,t}$ in (56) (as explained above, also $\eta^{(k)}_{n,t}$ can be expanded analogously to (57), with contributions associated to Feynman graphs similar to (58); the difference, of course, is that these contributions will depend on $\gamma_s^{(k+n)}$ for all $s \in [0,t]$, while (58) only depends on the initial data). Thus, we also obtain

$$\left|\mathrm{Tr} J^{(k)} \eta^{(k)}_{n,t}\right| \leq C^{k+n} t^{n/4}. \tag{62}$$

This bound immediately implies the uniqueness. In fact, given two solutions $\Gamma_{1,t} = \{\gamma^{(k)}_{1,t}\}_{k\geq 1}$ and $\Gamma_{2,t} = \{\gamma^{(k)}_{2,t}\}_{k\geq 1}$ of the infinite hierarchy (29), both satisfying the a-priori bounds (47) and with the same initial data, we can expand both in a Duhamel series of order n as in (54). If we fix $k \geq 1$, and consider the difference between $\gamma^{(k)}_{1,t}$ and $\gamma^{(k)}_{2,t}$, all terms (55) cancel out because they only depend on the initial data. Therefore, from (62), we immediately obtain that, for arbitrary (sufficiently smooth) compact k-particle operators $J^{(k)}$,

$$\left|\mathrm{Tr} J^{(k)} (\gamma^{(k)}_{1,t} - \gamma^{(k)}_{2,t})\right| \leq 2C^{k+n} t^{n/4}.$$

Since it is independent of n, the left side has to vanish for all $t < 1/C^4$. This proves uniqueness for short times. But then, since the a-priori bounds hold uniformly in time, the argument can be repeated to prove uniqueness for all times.

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Locality Estimates for Quantum Spin Systems

Bruno Nachtergaele and Robert Sims

Abstract We review some recent results that express or rely on the locality properties of the dynamics of quantum spin systems. In particular, we present a slightly sharper version of the recently obtained Lieb-Robinson bound on the group velocity for such systems on a large class of metric graphs. Using this bound we provide expressions of the quasi-locality of the dynamics in various forms, present a proof of the Exponential Clustering Theorem, and discuss a multi-dimensional Lieb-Schultz-Mattis Theorem.

1 Introduction

Locality is a fundamental property of all current physical theories. Sets of observables can be associated with points or bounded regions in space or space-time and a relativistic dynamics will preserve this structure [7]. How the locality property manifests itself mathematically in important situations continues to be an active topic of investigation [12].

There is a wide range of important physical systems, however, which we prefer to describe by very effective non-relativistic quantum theories with Hamiltonian dynamics. Even if the Hamiltonian has only finite-range interactions, the dynamics it generates generally does not preserve locality, i.e., there is no strict equivalent to the finite speed of light. However, locality still holds in an approximate sense, and there is an associated finite velocity, which is sometimes referred to as the group velocity. We call it the Lieb-Robinson velocity since Lieb and Robinson were the

Bruno Nachtergaele
Department of Mathematics, University of California, Davis, CA 95616, USA,
e-mail: bxn@math.ucdavis.edu

Robert Sims
Department of Mathematics, University of Arizona, Tucson, AZ 85721, USA,
e-mail: rsims@math.arizona.edu

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first to prove its existence and to obtain a bound for it [14]. They proved that to a high degree of accuracy locality is preserved by quantum spin dynamics in the sense that any local observable evolved for a time $t > 0$ remains localized in a region of space with diameter proportional to t, up to an arbitrarily small correction. This also means that spatial correlations between observables separated by a distance d cannot be established faster than a time of order d.

The fundamental issue of locality may be sufficient motivation to extend the Lieb-Robinson bounds to more general situations, but there are other good reasons to try to generalize their result and to improve the estimates they obtained. As we will discuss below, locality, or the approximate locality of the dynamics, has been shown to be responsible for a considerable number of other important properties relevant for models of many-body systems. In many situations, however, the implications of locality have yet to be fully explored.

We will begin this note by presenting a short proof of the new Lieb-Robinson bounds obtained successively in [18, 10], and [21]. This improved result we give below sharpens the bounds previously obtained in that the prefactor now only grows as the smallest surface area of the supports of the local observables. We do this in Sect. 2. An application where this surface area dependence, rather than volume dependence, is important can be found in [5].

In Sect. 3, we present two perspectives on how Lieb-Robinson bounds may be used to provide explicit estimates on the local structure of the time evolution. As a consequence, one easily derives bounds on, for example, multiple commutators and the rate at which spatial correlations can be established in normalized product states.

Section 4 discusses the so-called Exponential Clustering Theorem. In the relativistic context it has been known for a long time that a gap in the spectrum above the vacuum state implies exponential decay of spatial correlations in that state [3, 23, 6]. That a similar result should hold in the non-relativistic setting such as quantum spin systems was long expected and taken for granted by theoretical physicists [24]. In [9], Hastings proposed to use Lieb-Robinson bounds to obtain such a result and a complete proof was recently given in [18, 10].

As a final application of these locality bounds, we describe a new proof of the Lieb-Schultz-Mattis theorem, see [9, 19], in Sect. 5. These results can be traced back to [9] where Hastings introduced a new way to construct and analyze variational states for low-lying excitations of gapped Hamiltonians. He developed a notion of a *quasi-adiabatic evolution* [11] which he then used to present a multi-dimensional analogue of the celebrated Lieb-Schultz-Mattis theorem [15]. Such a theorem is applicable, for example, to the standard spin-1/2, anti-ferromagnetic Heisenberg model and yields an upper bound on the first excited state of order $c(\log L)/L$ for systems of size L. His arguments rely on Lieb-Robinson bounds and the Exponential Clustering Theorem in an essential way, and we have recently obtained a rigorous proof of this result which holds in a rather general setting, see [19].

We expect that the ideas currently emerging from recent applications of Lieb-Robinson bounds will continue to lead to interesting new results for quantum spin systems in the near future.

2 Lieb-Robinson Bounds

The first proof of locality bounds in the context of quantum spin systems appeared in 1972 in a paper by Lieb and Robinson [14]. They proved a bound on the group velocity corresponding to the dynamics generated by a variety of short range Hamiltonians. In a series of works [18, 10], and [21], these estimates have been generalized, and the proof we provide below, see Theorem 1, illustrates many of the new insights which have recently been developed.

The result stated in Theorem 1 below differs from that which may be found in [14] in two important ways. First, the new proof does not require the use of the Fourier transform, and therefore, it extends to models defined on sets without an underlying lattice structure. These results may be of interest to those who wish to study quantum spin systems in the context of quasi-crystals or in the study of circuits for quantum computation. Second, and most importantly, the constants which appear in our bound do not depend on the dimensions of the underlying, single-site Hilbert spaces. This opens up the possibility of applying them to models with an infinite-dimensional Hilbert space, such as lattice oscillators [22].

The basic set up in this theory concerns quantum spins systems, in particular, a finite or infinite number of spins labeled by $x \in V$. A finite dimensional Hilbert space $\mathscr{H}_x$ is assigned to each site $x \in V$. These may represent the spin of an electron, photon, or an atom. In other contexts, these states may represent the ground state and first exited state of an atom or a molecule. More abstractly, these systems may, for example, model a collection qubits, the basic units of quantum information theory and quantum computation.

If the set V is finite, the Hilbert space of states is given by $\mathscr{H}_V = \bigotimes_{x\in V} \mathscr{H}_x$. For each spin x, the observables are the complex $n_x \times n_x$ matrices, M_{n_x}, where $n_x = \dim(\mathscr{H}_x)$. In this context, the algebra of observables for the whole system is $\mathscr{A}_V = \bigotimes_{x\in V} M_{n_x}$.

The locality results we wish to describe pertain to observables with finite support. Here, the support of an observable is understood as follows. If $X \subset V$, we write $\mathscr{A}_X = \bigotimes_{x\in X} M_{n_x}$. By identifying $A \in \mathscr{A}_X$ with $A \otimes \mathbb{1} \in \mathscr{A}_V$, we have that $\mathscr{A}_X \subset \mathscr{A}_V$. The support of an observable $A \in \mathscr{A}_V$ in the minimal set $X \subset V$ for which $A = A' \otimes \mathbb{1}$ with $A' \in \mathscr{A}_X$.

For infinite V, the algebra of observables is the completion of the algebra of local observables given by

$$\mathscr{A}_V = \bigcup_{X\subset V} \mathscr{A}_X$$

where the union is over all finite $X \subset V$.

To describe the models we wish to investigate, we must first define interactions, local Hamiltonians, and the corresponding dynamics. An interaction is a map Φ from the set of subsets of V to $\mathscr{A}_V$ with the property that $\Phi(X) \in \mathscr{A}_X$ and $\Phi(X) = \Phi(X)^*$ for all finite $X \subset V$. A quantum spin model is defined by a family of local Hamiltonians, parametrized by finite subsets $\Lambda \subset V$, given by

$$H_\Lambda^\Phi = \sum_{X \subset \Lambda} \Phi(X). \tag{1}$$

For notational convenience, we will often drop the dependence of H_Λ^Φ on Φ. The dynamics, or time evolution, generated by a quantum spin model is the one-parameter group of automorphisms, $\{\tau_t^\Lambda\}_{t\in\mathbb{R}}$, defined by

$$\tau_t^\Lambda(A) = e^{itH_\Lambda} A e^{-itH_\Lambda}, \quad A \in \mathscr{A}_\Lambda, \tag{2}$$

which is always well defined for finite sets Λ. In the context of infinite systems, a boundedness condition on the interaction is required in order for the finite-volume dynamics to converge to a strongly continuous one-parameter group of automorphisms on $\mathscr{A}_V$.

The locality results we prove in Theorem 1 are valid for a large class of interactions. To describe this class precisely, we first put a condition on the set V, which is relevant only in the event that V is infinite. We assume that the set V is equipped with a metric d and that there exists a non-increasing function $F : [0, \infty) \to (0, \infty)$ for which:

(i) F is uniformly integrable over V, i.e.,

$$\|F\| = \sup_{x\in V} \sum_{y\in V} F(d(x, y)) < \infty, \tag{3}$$

and

(ii) F satisfies

$$C = \sup_{x,y\in V} \sum_{z\in V} \frac{F(d(x, z))F(d(z, y))}{F(d(x, y))} < \infty. \tag{4}$$

Given such a set V, it is easy to see that for any F which satisfies (i) and (ii) above, then the family of functions F_a, for $a \geq 0$, defined by

$$F_a(x) = e^{-ax} F(x), \tag{5}$$

also satisfy i) and ii) with $\|F_a\| \leq \|F\|$ and $C_a \leq C$. In this context, we define the set $\mathscr{B}_a(V)$ to be those interactions Φ on V which satisfy

$$\|\Phi\|_a = \sup_{x,y\in V} \sum_{X\ni x,y} \frac{\|\Phi(X)\|}{F_a(d(x, y))} < \infty. \tag{6}$$

The Lieb-Robinson bounds we will prove are valid for all $\Phi \in \mathscr{B}_a(V)$ with $a \geq 0$. Simply stated, these results correspond to estimates of the form

$$\|[\tau_t^\Lambda(A), B]\| \leq c(A, B)e^{-\mu(d(A,B)-v_\Phi|t|)}, \tag{7}$$

where A and B are local observables, $\tau_t^\Lambda(\cdot)$ is the time evolution corresponding to a finite volume Hamiltonian generated by an interaction $\Phi \in \mathscr{B}_a(V)$, and $d(A, B)$

is the distance between the supports of A and B. What is crucial in these estimates is that the constants $c(A, B)$, μ, and v_Φ are independent of the volume $\Lambda \subset V$ on which $\tau_t^\Lambda(\cdot)$ is defined. Physically, the constant v_Φ corresponds to a bound on the velocity at which the dynamics, generated by Φ, propagates through the system.

Intuitively, it is clear that the spread of the interactions through the system should depend on the surface area of the support of the local observable A, typically denoted by X, not it's volume. To make this explicit in our bound, we will denote the surface of a set X, regarded as a subset of $\Lambda \subset V$, by

$$S_\Lambda(X) = \{Z \subset \Lambda : Z \cap X \neq \emptyset \text{ and } Z \cap X^c \neq \emptyset\}. \tag{8}$$

Here we will use the notation $S(X) = S_V(X)$, and define

$$\|\Phi\|_a(x; X) = \begin{cases} \sup_{y\in\Lambda} \sum_{\substack{Z\in S(X):\\ x,y\in Z}} \frac{\|\Phi(Z)\|}{F_a(d(x,y))} & \text{if } x \in X, \\ 0 & \text{otherwise,} \end{cases} \tag{9}$$

a quantity corresponding to the interaction terms across the surface of X. Comparing the local quantity appearing in (9) with the norm on the full interaction given by (6), one trivially has that

$$\|\Phi\|_a(x; X) \leq \|\Phi\|_a \chi_{\partial_\Phi X}(x), \tag{10}$$

where we have used χ_Y to denote the characteristic function of a set $Y \subset \Lambda$, and we have introduced the Φ-boundary of a set X, written $\partial_\Phi X$, given by

$$\partial_\Phi X = \{x \in X : \exists Z \in S(X) \text{ with } x \in Z \text{ and } \Phi(Z) \neq 0\}. \tag{11}$$

The Lieb-Robinson bound may be stated as follows.

Theorem 1 (Lieb-Robinson Bound). *Let $a \geq 0$ and take $\Phi \in \mathscr{B}_a(V)$. For any finite set $\Lambda \subset V$, denote by $\tau_t^\Lambda(\cdot)$ the time evolution corresponding to the local Hamiltonian*

$$H_\Lambda = \sum_{Z\subset\Lambda} \Phi(Z). \tag{12}$$

Given any pair of local observables $A \in \mathscr{A}_X$ and $B \in \mathscr{A}_Y$ with $X, Y \subset \Lambda$ and $d(X, Y) > 0$, one may estimate

$$\|[\tau_t^\Lambda(A), B]\| \leq \frac{2\|A\|\|B\|}{\|\Phi\|_a C_a}(e^{2\|\Phi\|_a C_a|t|} - 1) D_a(X, Y), \tag{13}$$

for any $t \in \mathbb{R}$. Here the function $D_a(X, Y)$ is given by

$$D_a(X, Y) = \min\left[\sum_{x\in X}\sum_{y\in Y} \|\Phi\|_a(x; X) F_a(d(x, y)), \sum_{x\in X}\sum_{y\in Y} \|\Phi\|_a(y; Y) F_a(d(x, y))\right]. \tag{14}$$

A number of comments are useful in interpreting this theorem. First, we note that if X and Y have a non-empty intersection, then the argument provided below

produces an analogous bound with the factor $e^{2\|\Phi\|_a C_a|t|} - 1$ replaced by $e^{2\|\Phi\|_a C_a|t|}$. In the case of empty intersection and for small values of $|t|$, (13) is a better and sometimes useful estimates than the obvious bound $\|[\tau_t(A), B]\| \leq 2\|A\|\|B\|$, valid for all $t \in \mathbb{R}$.

Next, if $\Phi \in \mathscr{B}_a(V)$ for some $a > 0$, then one has the trivial estimate that

$$D_a(X, Y) \leq \|F_0\|\|\Phi\|_a \min(|\partial_\Phi X|, |\partial_\Phi Y|)e^{-ad(X,Y)}. \tag{15}$$

Clearly then, we have that

$$\|[\tau_t^\Lambda(A), B]\| \leq \frac{2\|A\|\|B\|\|F_0\|}{C_a} \min(|\partial_\Phi X|, |\partial_\Phi Y|)e^{-a[d(X,Y) - \frac{2\|\Phi\|_a C_a}{a}|t|]}, \tag{16}$$

which corresponds to a bound on the velocity of propagation given by

$$v_\Phi \leq \inf_{a>0} \frac{2\|\Phi\|_a C_a}{a}. \tag{17}$$

Next, we observe that for fixed local observables A and B, the bounds above, (13) and (16), are independent of the volume $\Lambda \subset V$; given that Λ contains the supports of both A and B. Furthermore, we note that these bounds only require that one of the observables has finite support; in particular, if $|X| < \infty$ and $d(X, Y) > 0$, then the bounds are valid irrespective of the support of B.

Proof (of Theorem 1). To prove (13), we will provide an estimate on the quantity

$$C_B(Z; t) = \sup_{A \in \mathscr{A}_Z} \frac{\|[\tau_t^\Lambda(A), B]\|}{\|A\|}, \tag{18}$$

where B is a fixed observable with support in Y, and the subset $Z \subset \Lambda$ we regard as arbitrary. Introduce the function

$$f(t) = \big[\tau_t^\Lambda(\tau_{-t}^X(A)), B\big], \tag{19}$$

where A and B are as in the statement of the theorem. Due to the strict locality of the Hamiltonian H_X, as defined e.g. in (12) and the fact that the observable $A \in \mathscr{A}_X$, we have that $\mathrm{supp}(\tau_{-t}^X(A)) \subset X$ for all $t \in \mathbb{R}$. It is straight forward to verify that

$$f'(t) = i \sum_{Z \in S_\Lambda(X)} \big[\tau_t^\Lambda(\Phi(Z)), f(t)\big] - i \sum_{Z \in S_\Lambda(X)} \big[\tau_t^\Lambda(\tau_{-t}^X(A)), \big[\tau_t^\Lambda(\Phi(Z)), B\big]\big]. \tag{20}$$

Since the first term in (20) is norm preserving, we find that

$$\big\|[\tau_t^\Lambda(\tau_{-t}^X(A)), B]\big\| \leq \|[A, B]\| + 2\|A\| \sum_{Z \in S(X)} \int_0^t \big\|[\tau_s^\Lambda(\Phi(Z)), B]\big\| ds. \tag{21}$$

The inequality (21) and the fact that $\|\tau_{-t}^X(A)\| = \|A\|$ together imply that

$$C_B(X;t) \leq C_B(X;0) + 2 \sum_{Z \in S(X)} \|\Phi(Z)\| \int_0^{|t|} C_B(Z;s) ds. \tag{22}$$

It is clear from the definition, see (18), that for any finite $Z \subset \Lambda$,

$$C_B(Z;0) \leq 2\|B\| \delta_Y(Z) \tag{23}$$

where $\delta_Y(Z) = 0$ if $Z \cap Y = \emptyset$ and $\delta_Y(Z) = 1$ otherwise. Using this fact, iteration of (22) yields that

$$C_B(X,t) \leq 2\|B\| \sum_{n=0}^{\infty} \frac{(2|t|)^n}{n!} a_n, \tag{24}$$

where for $n \geq 1$,

$$a_n = \sum_{Z_1 \in S(X)} \sum_{Z_2 \in S(Z_1)} \cdots \sum_{Z_n \in S(Z_{n-1})} \delta_Y(Z_n) \prod_{i=1}^{n} \|\Phi(Z_i)\|. \tag{25}$$

For an interaction $\Phi \in \mathscr{B}_a(V)$, one may estimate that

$$a_1 \leq \sum_{x \in X} \sum_{y \in Y} \sum_{\substack{Z \in S(X): \\ x,y \in Z}} \|\Phi(Z)\| \leq \sum_{x \in X} \sum_{y \in Y} \|\Phi\|_a(x;X) F_a(d(x,y)). \tag{26}$$

In addition,

$$\begin{aligned} a_2 &\leq \sum_{x \in X} \sum_{y \in Y} \sum_{z \in \Lambda} \sum_{\substack{Z_1 \in S(X): \\ x,z \in Z_1}} \|\Phi(Z_1)\| \sum_{\substack{Z_2 \in S(Z_1): \\ z,y \in Z_2}} \|\Phi(Z_2)\| \\ &\leq \|\Phi\|_a \sum_{x \in X} \sum_{y \in Y} \sum_{z \in \Lambda} F_a(d(z,y)) \sum_{\substack{Z_1 \in S(X): \\ x,z \in Z_1}} \|\Phi(Z_1)\| \\ &\leq \|\Phi\|_a \sum_{x \in X} \sum_{y \in Y} \sum_{z \in \Lambda} F_a(d(x,z)) F_a(d(z,y)) \|\Phi\|_a(x;X) \\ &\leq \|\Phi\|_a C_a \sum_{x \in X} \sum_{y \in Y} \|\Phi\|_a(x;X) F_a(d(x,y)), \end{aligned} \tag{27}$$

where we have used (4) for the final inequality. With analogous arguments, one finds that for all $n \geq 1$,

$$a_n \leq (\|\Phi\|_a C_a)^{n-1} \sum_{x \in X} \sum_{y \in Y} \|\Phi\|_a(x;X) F_a(d(x,y)). \tag{28}$$

Inserting (28) into (24) we see that

$$C_B(X,t) \leq \frac{2\|B\|}{\|\Phi\|_a C_a} (e^{2\|\Phi\|_a C_a |t|} - 1) \sum_{x \in X} \sum_{y \in Y} \|\Phi\|_a(x;X) F_a(d(x,y)), \tag{29}$$

from which (13) immediately follows. □

3 Quasi-Locality of the Dynamics

The Lieb-Robinson bounds of Theorem 1 imply that the dynamics of quantum lattice systems, those generated by short range interactions, are *quasi-local* in the sense that the diameter of the support of any evolved local observable does not grow faster than linearly with time, up to an arbitrarily small error. There are at least two interesting ways to give precise meaning to this quasi- locality property of the dynamics. In the first, one shows that the time-evolved observable can be well-approximated in norm by one with a strictly local support. This is achieved by the quantum version of integrating out the variables in the complement of a ball with a radius proportional to time. In the second, we show that to compute the dynamics up to a time $t > 0$, one can replace the Hamiltonian with a local Hamiltonian supported in a ball of radius proportional to t. Clearly, the net result is the same: the support of observables evolved with approximate dynamics remains contained in the ball where the local Hamiltonian is supported. After presenting the details of these two approaches, we conclude this section with a few interesting applications that immediately follow from quasi-locality.

As in the previous section, we will work with an interaction $\Phi \in \mathscr{B}_a(V)$ with $a > 0$. For the purpose of the discussion below, we will consider a finite subset $\Lambda \subset V$ and restrict our attention to the dynamics $\tau_t^\Lambda(\cdot)$ generated by the finite volume Hamiltonian H_Λ as defined in (1); our bounds will be independent of the volume Λ. For any $X \subset \Lambda$ we will denote by $X^c = \Lambda \setminus X$.

In the first approach to obtaining a local approximation with support contained in $X \subset \Lambda$, one takes the normalized partial trace over the Hilbert space associated with X^c. In order to estimate the norm difference it is convenient to calculate the partial trace as an integral over the group of unitaries [4]. Given an arbitrary observable $A \in \mathscr{A}_\Lambda$ and a set $X \subset \Lambda$, define

$$\langle A \rangle_{X^c} = \int_{\mathscr{U}(X^c)} U^* A U \mu(dU), \tag{30}$$

where $\mathscr{U}(X^c)$ denotes the group of unitary operators over the Hilbert space $\mathscr{H}_{X^c}$ and μ is the associated, normalized Haar measure. It is easy to see that for any $A \in \mathscr{A}_\Lambda$, the quantity $\langle A \rangle_{X^c}$ has been localized to X in the sense that $\langle A \rangle_{X^c} \in \mathscr{A}_X$. Moreover, the difference may be written in terms of a commutator, i.e. as

$$\langle A \rangle_{X^c} - A = \int_{\mathscr{U}(X^c)} U^* [A, U] \mu(dU). \tag{31}$$

To localize the dynamics, let $A \in \mathscr{A}_X$ and fix $\epsilon > 0$. Based on our estimates in Theorem 1, we approximate the support of $\tau_t^\Lambda(A)$ with a time-dependent ball

$$B_t(\epsilon, A) = \left\{ x \in \Lambda : d(x, X) \leq \frac{2\|\Phi\|_a C_a}{a} |t| + \epsilon \right\}. \tag{32}$$

For any unitary $U \in \mathscr{U}(B_t(\epsilon, A)^c)$, we clearly have that

$$d(X, \mathrm{supp}(U)) \geq \frac{2\|\Phi\|_a C_a}{a}|t| + \epsilon, \tag{33}$$

and therefore, using (31) above and our bound (16), we immediately conclude that

$$\begin{aligned}\left\|\tau_t^{\Lambda}(A) - \langle \tau_t^{\Lambda}(A)\rangle_{B_t(\epsilon,A)^c}\right\| &\leq \int_{\mathscr{U}(B_t^c(\epsilon))} \left\|\left[\tau_t^{\Lambda}(A), U\right]\right\| \mu(dU) \\ &\leq \frac{2\|A\||\partial_\Phi X|}{C_a}\|F_0\| e^{-a\epsilon}. \end{aligned} \tag{34}$$

The tolerance $\epsilon > 0$ can be chosen to optimize estimates.

In the second approach, one shows that only those terms in the Hamiltonian supported in $B_T(\epsilon, A)$ contribute significantly to the time evolution of A up to time T [21]. Again, we consider the finite volume dynamics applied to a local observable $A \in \mathscr{A}_X$. Fix $\epsilon > 0$, $T > 0$, and consider the ball $B_T(\epsilon, A)$ as defined in (32) above. The estimate

$$\left\|\tau_t^{\Lambda}(A) - \tau_t^{B_T(\epsilon,A)}(A)\right\| \leq \frac{\|A\|\|F_0\||\partial_\Phi X|}{C_a^2}(C_a + \|F_a\|)e^{-a\epsilon}, \tag{35}$$

valid for all $|t| \leq T$, readily follows from the results in [21]. In fact, the proof of (35) uses the following basic estimate, see e.g. Lemma 3.3 in [21],

Lemma 2. *Let $\Phi \in \mathscr{B}_a(V)$ with $a > 0$ and take a finite subset $\Lambda \subset V$. If the finite volume Hamiltonian is written as the sum of two self-adjoint operators, $H_\Lambda = H_\Lambda^{(1)} + H_\Lambda^{(2)}$, and for $i = 1, 2$, $\tau_t^{(i)}(\cdot)$ denotes the dynamics corresponding to $H_\Lambda^{(i)}$, then the following estimate is valid:*

$$\left\|\tau_t^{\Lambda}(A) - \tau_t^{(1)}(A)\right\| \leq \int_0^{|t|} \left\|\left[H_\Lambda^{(2)}, \tau_s^{(1)}(A)\right]\right\| ds, \tag{36}$$

for any observable A and $t \in \mathbb{R}$.

To apply Lemma 2 in the context discussed above, we write the local Hamiltonian as the sum of two terms:

$$H_\Lambda = \sum_{\substack{Z\subset\Lambda:\\ Z\notin S_\Lambda(B_T(\epsilon,A))}} \Phi(Z) + \sum_{\substack{Z\subset\Lambda:\\ Z\in S_\Lambda(B_T(\epsilon,A))}} \Phi(Z) = H_\Lambda^{(1)} + H_\Lambda^{(2)}. \tag{37}$$

Recall that for any $X \subset \Lambda$, we defined $S_\Lambda(X)$, the surface across X in Λ, with (8). Dropping the surface terms comprising $H_\Lambda^{(2)}$ above, decouples the dynamics, i.e., $\tau_t^{(1)}(A) = \tau_t^{B_T(\epsilon,A)}(A)$, and we find that for any $|t| \leq T$,

$$\left\|\tau_t^{\Lambda}(A) - \tau_t^{B_T(\epsilon,A)}(A)\right\| \leq \sum_{\substack{Z\in\Lambda:\\ Z\in S_\Lambda(B_T(\epsilon,A))}} \int_0^{|t|} \left\|\left[\Phi(Z), \tau_s^{B_T(\epsilon,A)}(A)\right]\right\| ds. \tag{38}$$

For each of the terms on the right hand side above, the Lieb-Robinson estimates imply that

$$\left\|\left[\Phi(Z), \tau_s^{B_T(\epsilon,A)}(A)\right]\right\| \leq \frac{2\|\Phi(Z)\|\|A\|}{C_a} e^{2\|\Phi\|_a C_a|s|} \sum_{z\in Z} \sum_{x\in\partial_\Phi X} F_a(d(x,z)). \quad (39)$$

Careful consideration of the combinatorics of these sums, exactly as done in [21], yields (35) as claimed.

It is interesting to ask about locality bounds for complex times. For one-dimensional systems with finite range interactions, Araki proved that the support does not grow faster than an exponential in $|z|$, where z is the complex time [2, Theorem 4.2]. In other words, the complex time evolution

$$\tau_z^{[-R,R]}(A) = e^{izH_\Lambda} A e^{-izH_\Lambda}$$

can be approximated by $\tau_z^{[-N,N]}(A)$ with small error, uniformly in R, as long as $\log|z| \leq cN$, for a suitable constant c. For stochastic dynamics of classical particle systems, good locality bounds that are very similar to Theorem 1 are known [16, Theorem 4.20]. Since these classical models with stochastic dynamics can be thought of as quantum systems, generated by particular Hamiltonians and evolving with purely imaginary times, this may indicate that the general result, which allows for no more than logarithmic growth of $|z|$, should not be considered the final word on this issue in regards to specific models of interest.

The quasi-locality formulation of the Lieb-Robinson bounds makes it easy to derive bounds on double and higher order commutators of the form

$$[\tau_{t_1}(A), [\tau_{t_2}(B), \tau_{t_3}(C]].$$

Such commutators remain small in norm as long as t_1, t_2, and t_3 are such that the intersection of the time-dependent "quasi-supports" remains empty. That is whenever $t_1, t_2, t_3 \in \mathbb{R}$ are such that

$$B_{t_1}(\epsilon, A) \cap B_{t_2}(\epsilon, B) \cap B_{t_3}(\epsilon, C) = \emptyset.$$

Another immediate application of the quasi-locality property is a bound on the rate at which spatial correlations can be created by the dynamics starting from a product state. In [21], we proved the following.

Theorem 3. *Let $a > 0$, $\Phi \in \mathscr{B}_a(V)$, and take Ω to be a normalized product state. Given $X, Y \subset \Lambda$ with $d(X,Y) > 0$ and local observables $A \in \mathscr{A}_X$ and $B \in \mathscr{A}_Y$, the estimate*

$$|\langle\tau_t(AB)\rangle - \langle\tau_t(A)\rangle\langle\tau_t(B)\rangle| \leq 4\|A\|\|B\|\|F\|(|\partial_\Phi X| + |\partial_\Phi Y|)G_a(t)e^{-ad(X,Y)} \quad (40)$$

is valid for all $t \in \mathbb{R}$. Here, for any observable A, the expectation value of A in the state Ω is denoted by $\langle A\rangle = \langle\Omega, A\Omega\rangle$, and the function

$$G_a(t) = \frac{C_a + \|F_a\|}{C_a} \|\Phi\|_a \int_0^{|t|} e^{2\|\Phi\|_a C_a |s|} ds. \tag{41}$$

4 Exponential Clustering

As a second application of these locality bounds, we will present a proof of the Exponential Clustering Theorem, see Theorem 4 below, which improves on the estimates found in [18], see also [10]. The proof of exponential clustering demonstrates that models with a spectral gap above the ground state energy necessarily exhibit exponential decay of spatial correlations in their ground state. Such results have recently appeared in a variety of contexts, e.g. [18, 10]. Using valence bond states, as is done in [17], one can easily construct gapless models with exponentially decaying ground state correlations indicating that, in general, there is no converse to Theorem 4.

In the finite volume, the notion of a gapped Hamiltonian is clear. If the system is infinite, we express the gap condition in terms of the limiting dynamics, the existence of which is guaranteed by the Lieb-Robinson bounds as discussed above, by considering a representation of the system on a Hilbert space $\mathscr{H}$. This means that there is a representation $\pi : \mathscr{A}_V \to \mathscr{B}(\mathscr{H})$, and a self-adjoint operator H on $\mathscr{H}$ such that

$$\pi(\tau_t(A)) = e^{itH} \pi(A) e^{-itH}, \quad A \in \mathscr{A}_V. \tag{42}$$

We will assume that the representative operator H is non-negative and that there exists a vector $\Omega \in \mathscr{H}$ for which $H\Omega = 0$. We say that the system has a spectral gap in the representation if there exists $\delta > 0$ such that $\mathrm{spec}(H) \cap (0, \delta) = \emptyset$. In this case, the spectral gap, γ, is defined by

$$\gamma = \sup\{\delta > 0 \mid \mathrm{spec}(H) \cap (0, \delta) = \emptyset\}. \tag{43}$$

Let P_0 denote the orthogonal projection onto $\ker H$. From now on, we will work in this representation and simply write A instead of $\pi(A)$.

Theorem 4 (Exponential Clustering). *Let $a > 0$ and take $\Phi \in \mathscr{B}_a(V)$. Suppose that the dynamics corresponding to Φ on V can be represented by a Hamiltonian H with a gap $\gamma > 0$ above the ground state energy, as described above. Let Ω be a normalized ground state vector for H; i.e. satisfy $H\Omega = 0$ with $\|\Omega\| = 1$. Then, there exists a constant $\mu > 0$ such that for any local observables $A \in \mathscr{A}_X$ and $B \in \mathscr{A}_Y$ with $X, Y \subset V$ and $d(X, Y) > 0$ satisfying $P_0 B \Omega = P_0 B^* \Omega = 0$, the bound*

$$|\langle \Omega, A\tau_{ib}(B)\Omega \rangle| \leq C(A, B, \gamma) e^{-\mu d(X,Y)(1 + \frac{\gamma^2 b^2}{4\mu^2 d(X,Y)^2})} \tag{44}$$

is valid for all non-negative b satisfying $0 \leq b\gamma \leq 2\mu d(X, Y)$. One may take

$$\mu = \frac{a\gamma}{4\|\Phi\|_a C_a + \gamma}, \tag{45}$$

as well as a constant

$$C(A, B, \gamma) = \|A\|\|B\|\left[1 + \sqrt{\frac{1}{\mu d(X, Y)}} + \frac{2\|F_0\|}{\pi C_a} \min(|\partial_\Phi X|, |\partial_\Phi Y|)\right]. \quad (46)$$

Note that in the case of a non-degenerate ground state, the condition on B is equivalent to $\langle \Omega, B\Omega \rangle = 0$. In this case, the theorem with $b = 0$ becomes

$$|\langle \Omega, AB\Omega \rangle - \langle \Omega, A\Omega \rangle \langle \Omega, B\Omega \rangle| \leq C(A, B, \gamma) e^{-\mu d(X,Y)}, \quad (47)$$

which is the standard (equal-time) correlation function. For small $b > 0$, the estimate (44) can be viewed as a perturbation of (47). Moreover, for $b > 0$ large, there is a trivial bound

$$|\langle \Omega, A\tau_{ib}(B)\Omega \rangle| \leq \|A\|\|B\|e^{-b\gamma}. \quad (48)$$

Proof. (*of Theorem* 4) We will follow very closely the proof which appears in [18] and refer to it whenever convenient. Consider the function f given by

$$f(z) = \langle \Omega, A\tau_z(B)\Omega \rangle = \int_\gamma^\infty e^{izE} d\langle A^*\Omega, P_E B\Omega \rangle, \quad (49)$$

where we have used the spectral theorem and the fact that B projects off the ground state. It is clear that the function f defined in (49) is analytic in the upper half plane and has a continuous (and bounded) boundary value on the real axis. The quantity we wish to bound corresponds to $f(ib)$ for $b > 0$. The case $b = 0$ will follow by a limiting argument.

Since the boundary value of f on $\mathbb{R}$ is continuous, one may show by a limiting argument that for any $T > b$,

$$f(ib) = \frac{1}{2\pi i} \int_{\Gamma_T} \frac{f(z)}{z - ib} dz, \quad (50)$$

where Γ_T is the semi-circular contour from $-T$ to T (on the real axis) into the upper half plane. As is shown in [18], the fact that the Hamiltonian is gapped, see also (49), implies that the integral over the circular part of the contour vanishes in the limit as $T \to \infty$, and therefore we have the bound

$$|\langle \Omega, A\tau_{ib}(B)\Omega \rangle| = |f(ib)| \leq \limsup_{T\to\infty} \left| \frac{1}{2\pi i} \int_{-T}^{T} \frac{f(t)}{t - ib} dt \right|. \quad (51)$$

The proof is then complete once we estimate this integral over the real line. While this inequality is true for any value of $b > 0$, to get the desired estimate, we will have to choose $b > 0$ sufficiently small; see the comments following (64) below.

Let $\alpha > 0$. We will choose this free parameter later. Observe that one may write

$$f(t) = e^{-\alpha b^2}\left[f(t)e^{-\alpha t^2} + f(t)\left(e^{\alpha b^2} - e^{-\alpha t^2}\right)\right]. \quad (52)$$

Clearly then, the integral we wish to bound, the one on the right hand side of (51) above, can be estimated by

$$e^{-\alpha b^2}\left|\frac{1}{2\pi i}\int_{-T}^{T}\frac{f(t)e^{-\alpha t^2}}{t-ib}dt\right|+e^{-\alpha b^2}\left|\frac{1}{2\pi i}\int_{-T}^{T}\frac{f(t)(e^{\alpha b^2}-e^{-\alpha t^2})}{t-ib}dt\right|. \quad (53)$$

We will bound the absolute value of each of the integrals appearing in (53) separately; the prefactor $e^{-\alpha b^2}$ will be an additional damping made explicit by the choice of α.

To bound the first integral appearing in (53), we further divide the integrand into two terms. Note that

$$f(t)e^{-\alpha t^2}=\langle\Omega,\tau_t(B)A\Omega\rangle e^{-\alpha t^2}+\langle\Omega,[A,\tau_t(B)]\Omega\rangle e^{-\alpha t^2}. \quad (54)$$

By the spectral theorem, we have that

$$\frac{1}{2\pi i}\int_{-T}^{T}\frac{\langle\Omega,\tau_t(B)A\Omega\rangle e^{-\alpha t^2}}{t-ib}dt=\int_{\gamma}^{\infty}\frac{1}{2\pi i}\int_{-T}^{T}\frac{e^{-itE}e^{-\alpha t^2}}{t-ib}dt\,d\langle P_E B^*\Omega,A\Omega\rangle, \quad (55)$$

where we have used now that $B^*\Omega$ is also orthogonal to the ground state. Applying Lemma 5, stated below, to the inner integral above, we have that

$$\lim_{T\to\infty}\frac{1}{2\pi i}\int_{-T}^{T}\frac{e^{-itE}e^{-\alpha t^2}}{t-ib}dt=\frac{1}{2\sqrt{\pi\alpha}}\int_{0}^{\infty}e^{-bw}e^{-\frac{(w+E)^2}{4\alpha}}dw\le\frac{1}{2}e^{-\frac{\gamma^2}{4\alpha}}, \quad (56)$$

where for the final inequality above we used that $E\ge\gamma>0$, $\alpha>0$, and $b>0$. From this we easily conclude that

$$\limsup_{T\to\infty}\left|\frac{1}{2\pi i}\int_{-T}^{T}\frac{\langle\Omega,\tau_t(B)A\Omega\rangle e^{-\alpha t^2}}{t-ib}dt\right|\le\frac{\|A\|\|B\|}{2}e^{-\frac{\gamma^2}{4\alpha}}. \quad (57)$$

For the integral corresponding to the second term in (54), it is easy to see that

$$\left|\frac{1}{2\pi i}\int_{-T}^{T}\frac{\langle\Omega,[A,\tau_t(B)]\Omega\rangle e^{-\alpha t^2}}{t-ib}dt\right|\le\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{\|[A,\tau_t(B)]\|}{|t|}e^{-\alpha t^2}dt, \quad (58)$$

where we have taken advantage of the fact that $b>0$. To complete our estimate, we will introduce another free parameter $s>0$. Here we use the Lieb-Robinson bound, Theorem 1, for times $|t|\le s$ and a basic norm estimate otherwise. The result is that the right hand side of (58) is bounded from above by

$$\frac{2\|A\|\|B\|}{\pi\|\Phi\|_a C_a}D_a(X,Y)(e^{2\|\Phi\|_a C_a s}-1)+\frac{\|A\|\|B\|}{s\sqrt{\pi\alpha}}e^{-\alpha s^2}. \quad (59)$$

This completes the bound of the first integral appearing in (53).

Using again the spectral theorem, the second integral in (53) may be written as

$$\left| \int_{\gamma}^{\infty} \frac{1}{2\pi i} \int_{-T}^{T} \frac{e^{itE}(e^{\alpha b^2} - e^{-\alpha t^2})}{t - ib} dt d\langle A^* \Omega, P_E B \Omega \rangle \right|. \tag{60}$$

As is described in detail in [18], we find that for $E \geq \gamma$ and α chosen such that $\gamma \geq 2\alpha b$,

$$\lim_{T\to\infty} \frac{1}{2\pi i} \int_{-T}^{T} \frac{e^{itE}}{t - ib}(e^{\alpha b^2} - e^{-\alpha t^2}) dt \leq \frac{1}{2} e^{-\frac{\gamma^2}{4\alpha}}, \tag{61}$$

which produces an estimate (one analogous to the bound in (57) above) for (60).

All of our estimates above combine to demonstrate that the right hand side of (51) is bounded by

$$\|A\| \|B\| \left[e^{-\frac{\gamma^2}{4\alpha}} + \frac{2D_a(X,Y)}{\pi \|\Phi\|_a C_a} (e^{2\|\Phi\|_a C_a s} - 1) + \frac{1}{s\sqrt{\pi\alpha}} e^{-\alpha s^2} \right] \tag{62}$$

if α satisfies $\gamma \geq 2\alpha b$. The choice $\alpha = \gamma/2s$ yields:

$$\|A\| \|B\| e^{-\frac{\gamma s}{2}} \left[1 + \sqrt{\frac{2}{\pi\gamma s}} + \frac{2D_a(X,Y)}{\pi \|\Phi\|_a C_a} e^{(2\|\Phi\|_a C_a + \frac{\gamma}{2})s} \right] \tag{63}$$

As is demonstrated in (15), $D_a(X,Y)$ decays exponentially as $e^{-ad(X,Y)}$. In this case, if we choose s to be the solution of the equation

$$s(2\|\Phi\|_a C_a + \gamma/2) = ad(X,Y), \tag{64}$$

then we have proven the result. Notice that we have chosen α in terms of s, which is defined independently of b, thus the condition $\gamma \geq 2\alpha b$ will be satisfied for sufficiently small $b > 0$. □

In our proof of the Exponential Clustering Theorem above, we used several times the following useful fact, a proof of which appears in [18].

Lemma 5. *Let $E \in \mathbb{R}$, $\alpha > 0$, and $z \in \mathbb{C}^+ = \{z \in \mathbb{C} : Im[z] > 0\}$. One has that*

$$\lim_{T\to\infty} \frac{1}{2\pi i} \int_{-T}^{T} \frac{e^{iEt} e^{-\alpha t^2}}{t - z} dt = \frac{1}{2\sqrt{\pi\alpha}} \int_{0}^{\infty} e^{iwz} e^{-\frac{(w-E)^2}{4\alpha}} dw. \tag{65}$$

Moreover, the convergence is uniform for $z \in \mathbb{C}^+$.

5 The Lieb-Schultz-Mattis Theorem

As a final application of these locality bounds, in particular both Theorem 1 and Theorem 4, we were recently able to provide a rigorous proof the Lieb-Schultz-Mattis theorem, see [20], which is valid in arbitrary dimensions. In this section, we will discuss this result and outline the ideas which motivate our proof.

5.1 The Result and Some Words on the Proof

The classical Lieb-Schultz-Mattis Theorem (LSM), [15], concerns the spin-1/2, anti-ferromagnetic Heisenberg chain. This model is defined through a family of Hamiltonians H_L, acting on the Hilbert space $\mathscr{H}_{[1,L]} = \bigotimes_{x\in[1,L]} \mathbb{C}^2$, with the form

$$H_L = \sum_{x=1}^{L-1} \boldsymbol{S}_x \cdot \boldsymbol{S}_{x+1}. \tag{66}$$

Here, for each integer $x \in [1, L]$, the spin vectors $\boldsymbol{S}_x$ have components

$$S_x^j = \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes S^j \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}, \quad j = 1, 2, 3, \tag{67}$$

where S^j is the corresponding spin-1/2 (Pauli) matrix acting on the x-th factor of $\mathscr{H}_{[1,L]}$. The LSM Theorem may be stated as follows.

Theorem 6. *(LSM, 1961) If the ground state of H_L is unique, then the gap in energy between the ground state and the first excited state is bounded by C/L.*

A further result by Lieb and Mattis in 1966, [13], verified that under certain conditions, for example when L is even, the main assumption in the LSM Theorem, specifically the uniqueness of the ground state, is indeed satisfied. Almost twenty years later, the LSM Theorem was generalized to encompass a variety of other one (and quasi-one) dimensional models by Affleck and Lieb in [1]. In particular, this result applies to those chains of even length with spins having arbitrary half-integer magnitude. Note: Here and in the rest of this section the term half-integer, or half-integral, refers to one-half of a positive odd integer, i.e., an element of the set $\mathbb{N} + 1/2$.

For models to which the LSM Theorem applies, one expects that the excitation spectrum corresponding to the thermodynamic limit has no gap above the ground state energy. It is interesting to note that the predictions of Haldane [8] suggest that such a result is rather sensitive to the type of interaction terms. In fact, the spin-1, anti-ferromagnetic Heisenberg chain is predicted to have a robust gap above the ground state energy in the thermodynamic limit.

In a work of 2004, see [9], Hastings argued that a higher dimensional analogue of the LSM Theorem could be proven using the improved locality bounds which have recently been established. We will now summarize these ideas and indicate how they may be implemented to demonstrate a rigorous proof of this theorem.

The multi-dimensional LSM Theorem, stated as Theorem 7 below, is valid for a large class of models; a detailed proof of this is contained in [20]. For simplicity of presentation in this review article, we will restrict our attention to the spin-1/2, Heisenberg anti-ferromagnet, however, our general assumptions are discussed in Sect. 5.2.4. In ν dimensions, the model of interest is defined on subsets $V_L \subset \mathbb{Z}^\nu$ in analogy to (66) above, i.e. one considers Hamiltonians

$$H_L = \sum_{\substack{x,y\in V_L:\\ |x-y|=1}} \boldsymbol{S}_x \cdot \boldsymbol{S}_y \tag{68}$$

acting on the Hilbert space $\mathscr{H}_{V_L} = \bigotimes_{x\in V_L} \mathbb{C}^2$. It is easy to state the new result.

Theorem 7. *If the ground state of H_L is non-degenerate, then the gap, γ_L, above the ground state energy satisfies*

$$\gamma_L \leq C\frac{\log(L)}{L}. \tag{69}$$

The logarithmic correction which appears in Theorem 7, in contrast to the original result of Theorem 6, seems to be an inevitable consequence of the locality bounds we incorporate in our proof. It is an interesting open question to determine whether or not there is a class of models, in dimensions $\nu > 1$, for which one can prove such a bound without the logarithmic correction.

In essense, Theorem 7 is proven using a variational argument. Letting ψ_0 denote the unique, normalized ground state, we know that for any normalized vector ψ_1 with $|\langle\psi_0, \psi_1\rangle| \neq 1$, the bound

$$0 < \gamma \leq \frac{\langle\psi_1, (H - E_0)\psi_1\rangle}{1 - |\langle\psi_0, \psi_1\rangle|^2} \tag{70}$$

is always valid. Here we have dropped the dependence of all quantities on the length scale L. From this perspective, there are only three steps necessary to prove the desired result. First, we must construct a normalized trial state ψ_1, as indicated above. Next, we must estimate the difference in the energy corresponding to ψ_1 and E_0. Lastly, we must ensure that the inner product $|\langle\psi_0, \psi_1\rangle|$ remains sufficiently small.

This method of proof is complicated by the fact that the ground state is virtually unknown, and therefore the means by which one should construct a trial state is not a priori clear. Inspiration for the construction of our variational state comes from the work of Hastings, again see [9], in which he proposes to consider the ground state of a modified Hamiltonian, H_θ, where the interactions in a given hyperplane have been twisted by an angle of θ; more on this below. The ground state of this modified Hamiltonian may be regarded as the solution of a specific differential equation, in the variable θ, whose initial condition corresponds to the unique ground state whose existence we assumed. The solution of Hastings' differential equation is amenable to analysis, in particular, one can apply both the Lieb-Robinson bounds and the Exponential Clustering Theorem to provide the desired energy and orthogonality estimates mentioned above. One may recall that the clustering bounds, as in Theorem 4, provide estimates which themselves depend on the size of gap γ_L. For this reason, the argument proceeds by way of contradiction. In fact, by assuming that there exists a sufficiently large constant C for which the gap satisfies $\gamma_L > C\log(L)/L$ for large enough L, we construct a trial state whose energy eventually violates this bound.

5.2 A More Detailed Outline of the Proof

5.2.1 Constructing the Trial State

In our proof, we use the fact that the Hamiltonians we consider are assumed to have at least one direction of translation invariance. We incorporate this into our notation by considering finite subsets $V_L \subset \mathbb{Z}^\nu$ of the form $V_L = [1, L] \times V_L^\perp$ where we have isolated a particular direction, which we will often refer to as the horizontal direction, and perpendicular sets $V_L^\perp \subset \mathbb{Z}^{\nu-1}$ with cardinality $|V_L^\perp| \leq CL^{\nu-1}$. For the orthogonality result, we will also need to assume that $|V_L^\perp|$ is odd, see Sect. 5.2.3. The trial state is constructed from a perturbation of the Hamiltonian H_L defined by "twisting" certain interaction terms. A twist in the hyperplane situated at a site $m \in [1, L]$ is defined by replacing all interaction terms $\boldsymbol{S}_x \cdot \boldsymbol{S}_y$ in (68) corresponding to horizontal bonds with $x = (m, v)$, $y = (m + 1, v)$, and some $v \in V_L^\perp$ by terms of the form

$$h_{xy}(\theta) = \boldsymbol{S}_x \cdot e^{-i\theta S_y^3} \boldsymbol{S}_y e^{i\theta S_y^3} \tag{71}$$

for some $\theta \in \mathbb{R}$. A doubly twisted Heisenberg Hamiltonian is then given by

$$H_{\theta,\theta'} = \sum_{\substack{x,y \in V_L: \\ |x-y|=1}} h_{xy}(\theta_{xy}) \tag{72}$$

where

$$\theta_{xy} = \begin{cases} \theta, & \text{if } x = (m, v),\ y = (m + 1, v) \text{ for some } v \in V_L^\perp, \\ \theta', & \text{if } x = (m + L/2, v),\ y = (m + 1 + L/2, v) \text{ for } v \in V_L^\perp, \\ 0, & \text{otherwise.} \end{cases} \tag{73}$$

Here we have taken periodic boundary conditions in the horizontal direction.

It is interesting to note the behavior of the lowest eigenvalues of the singly twisted Heisenberg Hamiltonian $H_{\theta,0}$ for a simple spin ring with an even number of spins. The behavior depends in an interesting way on the magnitude of the spins. When the spins are half-integer, the two lowest eigenvalues cross at $\theta = \pi$. In contrast, when the spins are integer, they remain non-degenerate. The quasi-adiabatic evolution is a device designed to construct a continuous path from the ground state of $H_{0,0}$ to the first excited state of $H_{2\pi,0}$ which, of course, are both identical to the unperturbed Hamiltonian.

One of Hastings' crucial insights in [9] is that, for the half-integer spin case, the first excited state can be obtained by applying a "quasi-adiabatic evolution" to the ground state; here θ is the evolution parameter. More concretely, let $\psi_0(\theta, \theta')$ and $E_0(\theta, \theta')$ denote the ground state and ground state energy of the doubly twisted Hamiltonian $H_{\theta,\theta'}$, respectively. It is easy to see that along the path $\theta' = -\theta$, the Hamiltonian $H_{\theta,-\theta}$ is unitarily equivalent to the unperturbed Hamiltonian $H_L = H_{0,0}$. By differentiating the eigenvalue equation $H_{\theta,-\theta}\psi_0(\theta, -\theta) = E_0(\theta, -\theta) \times$

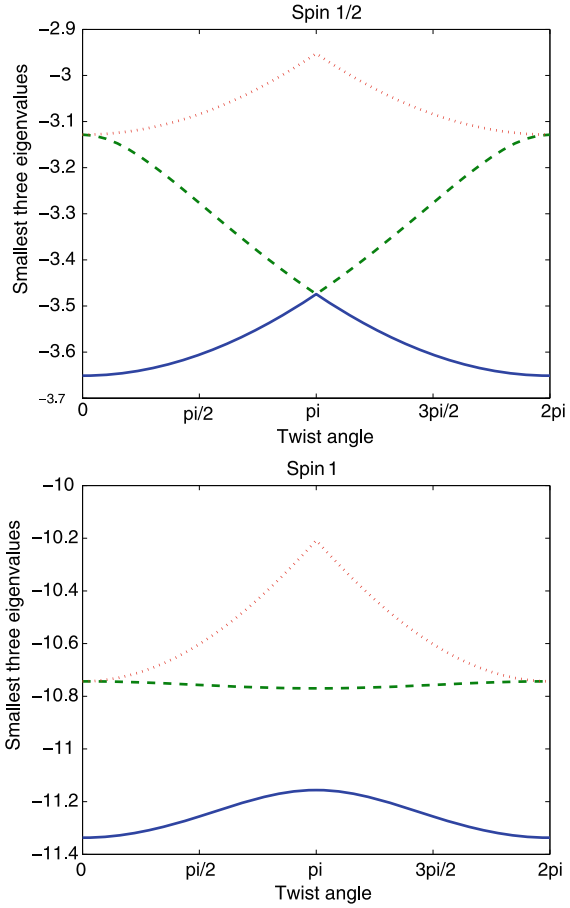

Fig. 1 Plot of the three lowest eigenvalues of $H_{\theta,0}$, the singly twisted Heisenberg Hamiltonian for a ring of 8 spins. The magnitude of spins is $S = 1/2$ in the plot on the left and $S = 1$ on the right

$\psi_0(\theta, -\theta)$ and using that $\partial_\theta E_0(\theta, -\theta) = 0$, one obtains

$$\partial_\theta \psi_0(\theta, -\theta) = -\frac{1}{H_{\theta,-\theta} - E_0}[\partial_\theta H_{\theta,-\theta}]\psi_0(\theta, -\theta). \tag{74}$$

Formally, (74) may be re-written using the Heisenberg dynamics as follows,

$$\partial_\theta \psi_0(\theta, -\theta) = B(\theta)\psi_0(\theta, -\theta), \tag{75}$$

where the operator $B(\theta)$ is defined by

$$B(\theta) = -\int_0^\infty \tau_{it}(\partial_\theta H_{\theta,-\theta}) P_0(\theta, -\theta) dt. \tag{76}$$

Here we have denoted by $\tau_t(\cdot)$ the dynamics generated by the Hamiltonian $H_{\theta,-\theta}$, and $P_0(\theta, -\theta)$ is the corresponding spectral projection onto the ground state. Due to the gap assumption, (76) is well-defined.

Equation (75) captures the evolution of the ground state of a doubly twisted Hamiltonian along the path $\theta' = -\theta$ where the effect of the first twist is canceled by the second. The trial state is obtained by using an approximation of the differential equation in (75) to describe the ground state of the singly twisted Hamiltonian $H_{\theta,0}$. Introduce the parameters $\alpha > 0$ and $T > 0$. To approximate the imaginary time evolution corresponding to an arbitrary Hamiltonian H, with dynamics $\tau_s(\cdot)$, at time $t > 0$, we define

$$A_\alpha(it, H) = \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \tau_s(A) \frac{e^{-\alpha s^2}}{s - it} ds \tag{77}$$

for any observable A. In general, an anti-Hermitian operator of the form

$$B_{\alpha,T}(A, H) = -\int_0^T [A_\alpha(it, H) - A_\alpha(it, H)^*] dt, \tag{78}$$

will be used in place of (76).

Note that the observable which is evolved in (76), $\partial_\theta H_{\theta,-\theta}$, contains terms of two types. The first are localized around the twist of angle θ which correspond to horizontal bonds (x, y) of the type $x = (m, v)$, $y = (m + 1, v)$, and some $v \in V_L^\perp$. The second are similar, yet localized around the twist of angle $-\theta$. We group these two types of terms together and write $\partial_\theta H_{\theta,-\theta} = \partial_1 H_{\theta,-\theta} - \partial_2 H_{\theta,-\theta}$ to simplify notation. By linearity, the operator

$$B_{\alpha,T}(\partial_\theta H_{\theta,-\theta}, H_{\theta,-\theta}) = B_{\alpha,T}(\partial_1 H_{\theta,-\theta}, H_{\theta,-\theta}) - B_{\alpha,T}(\partial_2 H_{\theta,-\theta}, H_{\theta,-\theta}). \tag{79}$$

Given a sufficiently large gap γ_L, there is a choice of the parameters α and T for which the ground state $\psi_0(\theta, -\theta)$ is well approximated by the solution of the differential equation (75) with $B(\theta)$ replaced by $B_{\alpha,T}(\partial_\theta H_{\theta,-\theta}, H_{\theta,-\theta})$. Hastings' clever proposal is that one may also approximate the ground state of the singly twisted Hamiltonian, $\psi_0(\theta, 0)$, by evolving with just the first term on the right hand side of (79) above. More concretely, consider the operator $B_{\alpha,T}(\theta)$ defined by setting $B_{\alpha,T}(\theta) = B_{\alpha,T}(\partial_1 H_{\theta,-\theta}, H_{\theta,-\theta})$ and solve the *Hastings' Equation* given by

$$\partial_\theta \psi_{\alpha,T}(\theta) = B_{\alpha,T}(\theta) \psi_{\alpha,T}(\theta) \tag{80}$$

with initial condition $\psi_{\alpha,T}(0) = \psi_0(0, 0)$, i.e., the ground state of the unperturbed Hamiltonian. Under the choice of parameters $\alpha = \gamma_L/L$ and $T = L/2$, the resulting variational state $\psi_1 = \psi_{\alpha,T}(2\pi)$ may be estimated in such a way that Theorem 7 follows. We note that a particularly nice feature of the differential equation (80) is that the operator $B_{\alpha,T}(\theta)$ is anti-Hermitian, and therefore the solution remains normalized for all $\theta \in [0, 2\pi]$. Hastings interprets the solution of (80) as a *quasi-adiabatic evolution* of the ground state $\psi_0 = \psi_0(0, 0)$.

5.2.2 Locality and the Trial State

One key technical lemma, which we use repeatedly in all of the estimates that follow, concerns the local evolution of the solution to (80). Consider a sub-volume $\Lambda_L(m) \subset V_L$ localized around the twist of angle θ, for example, take $\Lambda_L(m)$ to be of the form $[m-(L/4-2), m+(L/4-2)] \times V_L^{\perp}$ which is slightly less than half of the system. Let $\rho_{\alpha,T}(\theta)$ and $\rho_0(\theta, -\theta)$ denote the density matrices corresponding to the states $\psi_{\alpha,T}(\theta)$ and $\psi_0(\theta, -\theta)$.

Lemma 8. *Suppose there exists a constant $c > 0$ such that $L\gamma_L \geq c$ and choose $\alpha = \gamma_L/L$ and $T = L/2$. Then, there exists constants $C > 0$ and $k > 0$ such that*

$$\sup_{\theta\in[0,2\pi]} \left\| \mathrm{Tr}_{V_L\setminus\Lambda_L(m)}[\rho_{\alpha,T}(\theta) - \rho_0(\theta,-\theta)] \right\|_1 \leq CL^{2\nu}e^{-kL\gamma_L}.$$

Since the proof proceeds by way of contradiction, the assumption $L\gamma_L \geq c$ is part of the argument. Moreover, it is easy to produce a bound on γ_L from above that is independent of the length scale L. Lemma 8 demonstrates that if $L\gamma_L$ is sufficiently large, then the effect of ignoring the second twist in the definition of $\psi_{\alpha,T}(\theta)$ is negligible when one restricts their attention to observables localized in $\Lambda_L(m)$. The proof of this lemma uses both the Lieb-Robinson bound, Theorem 1, and the Exponential Clustering result, Theorem 4.

5.2.3 The Estimates

The Energy Estimate: To estimate the energy of the trial state, we consider the function

$$E(\theta) = \langle \psi_{\alpha,T}(\theta), H_{\theta,-\theta}\psi_{\alpha,T}(\theta)\rangle. \tag{81}$$

Due to the initial condition used to define $\psi_{\alpha,T}(\theta)$, we know that $E(0) = E_0$ the ground state energy, and since $H_{2\pi,-2\pi} = H_L$, $E(2\pi)$ corresponds to the energy of the trial state $\psi_1 = \psi_{\alpha,T}(2\pi)$. The main idea here is to use the locality property of the trial state, i.e. Lemma 8, and the unitary equivalence of the Hamiltonians $H_{\theta,-\theta}$ to obtain an estimate on the derivative of this function which is uniform for $\theta \in [0, 2\pi]$. Explicitly, we can prove the following result.

Theorem 9. *Suppose there exists a constant $c > 0$ such that $L\gamma_L \geq c$ and choose $\alpha = \gamma_L/L$ and $T = L/2$. Then, there exists constants $C > 0$ and $k > 0$ such that*

$$|\langle \psi_1, H_L\psi_1\rangle - E_0| \leq CL^{3\nu-1}e^{-kL\gamma_L}.$$

The Orthogonality Estimate: As we mentioned before, Hastings' quasi-adiabatic evolution is norm preserving. In particular, we are guaranteed that $\|\psi_1\| = \|\psi_0\| = 1$. Our argument that ψ_1 is sufficiently orthogonal to ψ_0 makes essential use of the fact that the total spin in each perpendicular set, $V_L^{\perp}$, is half-integer. In the case of the spin-1/2, anti-ferromagnetic Heisenberg model, this corresponds to the assumption that $|V_L^{\perp}|$ is odd. We have the following theorem.

Theorem 10. *Suppose there exists a constant $c > 0$ such that $L\gamma_L \geq c$ and choose $\alpha = \gamma_L/L$ and $T = L/2$. Then, there exists constants $C > 0$ and $k > 0$ such that*

$$|\langle \psi_1, \psi_0 \rangle| \leq CL^{2\nu} e^{-kL\gamma_L}.$$

To prove this result we observe that, although the ground state $\psi_0(\theta, -\theta)$ of the perturbed Hamiltonian is not translation invariant, it is invariant with respect to "twisted" translations. In fact, let T be a unitary implementing the translation symmetry in the horizontal direction, specifically the direction in which we have imposed periodic boundary conditions, chosen such that $T\psi_0 = \psi_0$. This is possible since ψ_0 is the unique ground state and the Hamiltonian is translation invariant with respect to T, i.e., $T^* H_L T = H_L$.

Define twisted translations by setting

$$T_{\theta,\theta'} = TU_m(\theta)U_{m+L/2}(\theta') \tag{82}$$

where the column rotation, $U_n(\theta)$, applies the rotation $e^{i\theta S_x^3}$ to all sites for the form $x = (n, v)$, for some $v \in V_L^{\perp}$. The unitary equivalence of the doubly twisted Hamiltonian $H_{\theta,-\theta}$ to $H_L = H_{0,0}$ can also be expressed in terms of these column rotations

$$H_{\theta,-\theta} = W(\theta)^* H_{0,0} W(\theta), \tag{83}$$

where

$$W(\theta) = \bigotimes_{m<n\leq m+L/2} U_n(\theta). \tag{84}$$

With these definitions, it is easy to see that $W(\theta)^* T W(\theta) = T_{\theta,-\theta}$ commutes with $H_{\theta,-\theta}$, and therefore,

$$T_{\theta,-\theta}\psi_0(\theta, -\theta) = \psi_0(\theta, -\theta), \tag{85}$$

as we claimed.

The main idea in the proof of Theorem 10 is to again use the locality properties of the solution of Hastings' Equation (80) to show that

$$T_{\theta,0}\psi_{\alpha,T}(\theta) \sim \psi_{\alpha,T}(\theta). \tag{86}$$

Since the total spin in each $V_L^{\perp}$ is half-integer, again a consequence of assuming $|V_L^{\perp}|$ is odd, the column rotation $U_m(2\pi) = -\mathbb{1}$. Clearly then, $T_{2\pi,0} = -T$, and therefore, $T\psi_1 \sim -\psi_1$. As we have chosen T so that, $T\psi_0 = \psi_0$, this implies that ψ_1 is nearly orthogonal to ψ_0.

5.2.4 Generalizations

As we previously indicated, the proof of the multi-dimensional Lieb-Schultz-Mattis Theorem, demonstrated in [20], applies to a large variety of models. In what follows

below, we will outline a list of assumptions which define a wide class of Hamiltonians for which the LSM Theorem remains valid.

The Basic Set-Up: It is not important for our argument that the underlying sets have a lattice structure, in particular the sets V_L need not be subsets of $\mathbb{Z}^\nu$. Rather, we need only assume that there is, at least, one direction of increase, which previously we labeled the horizontal direction. We make this notion concrete by assuming that there exists an increasing sequence of finite sets $\{V_L\}_{L\geq 1}$, exhausting some infinite set V, which are of the form $V_L = [1, L] \times V_L^\perp$. We also assume a bound on the cardinality of the perpendicular sets of the form $|V_L^\perp| \leq cL^\alpha$ for some $\alpha \geq 0$, and it is natural, but not necessary, to take $\alpha = \nu - 1$.

The interactions can also be of a general form. We assume that the set V is equipped with a metric d and a function F as described in Sect. 2. To start with, we work with interactions $\Phi \in \mathscr{B}_a(V)$ for some $a > 0$ so that the infinite volume dynamics is well defined from the beginning. In contrast to (68), the more general finite volume Hamiltonians are of the form

$$H_L = \sum_{X\subset V_L} \Phi(X) + \text{ boundary terms}, \tag{87}$$

where we will assume periodic boundary conditions in the horizontal direction and arbitrary boundary conditions in the other directions.

Assumption I. Our first assumption is that the interaction $\Phi \in \mathscr{B}_a(V)$ is translation invariant in the horizontal direction. This is clearly the case for the Heisenberg anti-ferromagnet, and in general, it means that for any $X \subset V_L$,

$$\Phi(X + e_1) = \alpha_1(\Phi(X)), \tag{88}$$

where $X + e_1$ is the translation of all points in X by one unit in the horizontal direction and $\alpha_1(\cdot)$ is the translation automorphism which maps $\mathscr{A}_{(n,V_L^\perp)}$ into $\mathscr{A}_{(n+1,V_L^\perp)}$ for all $n \in \mathbb{Z}$. Here the column sets $(n, V_L^\perp)$ are defined by $(n, V_L^\perp) = \{x \in V_L : x = (n, v) \text{ for some } v \in V_L^\perp\}$. Due to the assumed periodicity in the horizontal direction, this translation invariance can be implemented by a unitary $T \in \mathscr{A}_{V_L}$, i.e. $\Phi(X + e_1) = T^*\Phi(X)T$ for all $X \subset V_L$. This unitary T will depend on the length scale L, but we will suppress this in our notation.

Assumption II. We further assume that the interaction has a finite range $R > 0$ in the horizontal direction. This assumption is not strictly necessary. It is clear from the estimates in [20] that the result remains true even if the interactions are of long range with sufficiently fast decay.

Assumption III. We assume the interaction Φ has rotation invariance about one axis. Again, this is clearly the case for the Heisenberg model. In the more abstract setting, we specifically assume that for each $x \in V$ there is a local hermitian matrix, which we will denote by S_x^3, with eigenvalues that are either all integer or all half-integer. These matrices are also required to be translates of one another, i.e., for any $x \in V$, $\alpha_1(S_x^3) = S_{x+e_1}^3$. Rotation invariance for a general interaction Φ means that

for any $X \subset V_L$,

$$U^*(\theta)\Phi(X)U(\theta) = \Phi(X) \text{ for all } \theta \in \mathbb{R}, \tag{89}$$

where the rotation $U(\theta)$ is defined by

$$U(\theta) = \bigotimes_{x \in V_L} e^{i\theta S_x^3}. \tag{90}$$

Assumption IV. We assume that the matrices introduced above, i.e. S_x^3, are uniformly bounded in the sense that there exists a positive real number S for which $\sup_{x \in V} \|S_x^3\| \leq S$. In addition, we must assume an odd parity condition on the spins. Define the parity p_x of a site $x \in V$ to be 0 if the eigenvalues of S_x^3 are all integers and 1/2 if they are all half-integers. The odd parity assumption is that

$$\sum_{v \in V_L^\perp} p_{(n,v)} \in \mathbb{N} + 1/2, \tag{91}$$

for all $n \in \mathbb{Z}$. For the spin-1/2 Heisenberg model, we satisfied this assumption by taking the cardinality of the perpendicular sets, $|V_L^\perp|$, to be odd. In general, the sum of the spins over the perpendicular set needs to be half-integer to ensure that the column rotations $U_n(\theta)$, as defined after equation (82), satisfy $U_n(2\pi) = -\mathbb{1}$. As we have seen, such an identity plays a crucial role in our argument for orthogonality.

Assumption V. The ground state of H_L is assumed to be non-degenerate. In this case, it is also an eigenvector of the translation T and the rotations $U(\theta)$ introduced above. We assume that the ground state has eigenvalue one for both T and $U(\theta)$.

Assumption VI. We assume that there are orthonormal bases of the Hilbert spaces $\mathscr{H}_{V_L}$ with respect to which S_x^3 and $\Phi(X)$ are real for all $x \in V$ and all finite $X \subset V$. This assumption is satisfied by the Heisenberg model, and it is an important symmetry which allows us, in general, to prove that the ground state eigenvalue is invariant with respect to the doubly twisted Hamiltonian $H_{\theta,-\theta}$.

The following theorem was proven in [20].

Theorem 11. *Let $\Phi \in \mathscr{B}_a(V)$ for some $a > 0$. If Φ satisfies assumptions I-VI above, then the gap, γ_L, above the ground state energy of H_L satisfies*

$$\gamma_L \leq C\frac{\log(L)}{L}. \tag{92}$$

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On Resolvent Identities in Gaussian Ensembles at the Edge of the Spectrum

Alexander Soshnikov

Abstract We obtain the recursive identities for the joint moments of the traces of the powers of the resolvent for Gaussian ensembles of random matrices at the soft and hard edges of the spectrum. We also discuss the possible ways to extend these results to the non-Gaussian case.

1 Introduction

Consider the Gaussian Orthogonal Ensemble (GOE) of real symmetric $n \times n$ random matrices

$$A_n = \frac{1}{\sqrt{n}}(a_{ij})_{i,j=1}^{n}, \tag{1}$$

where $\{a_{ij} = a_{ji}\}_{i \le j}$ are independent $N(0, 1 + \delta_{ij})$ random variables. GOE is the archetypal example of a Wigner real symmetric random matrix where the matrix entries $\{a_{ij} = a_{ji}\}_{i \le j}$ are assumed to be independent up from the diagonal, centralized, and to have the same variance (except, possibly, on the diagonal). It follows from the classical Wigner semi-circle law [20, 21, 1] that the empirical distribution function of the eigenvalues of A_n converges as $n \to \infty$ to the limiting distribution with the probability density $\frac{1}{2\pi}\sqrt{4 - x^2}$ supported on the interval $[-2, 2]$. Celebrated work by Tracy and Widom (see [18] for the GOE case) proved that the largest eigenvalues of A_n deviate from the right edge of the spectrum on the order of $n^{-2/3}$. In particular, Tracy and Widom calculated the limiting distribution of the largest eigenvalue:

Alexander Soshnikov
Department of Mathematics, University of California at Davis, One Shields Ave., Davis, CA 95616, USA, e-mail: soshniko@math.ucdavis.edu

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$$\lim_{n\to\infty} \mathbb{P}\big(\lambda_{\max} \le 2 + xn^{-2/3}\big) = F_1(x) = \exp\left(-1/2 \int_x^\infty q(t) + (t-x)q^2(t)dt\right), \tag{2}$$

where $q(x)$ is the solution of the Painléve II differential equation $q''(x) = xq(x) + 2q^3(x)$ with the asymptotics at infinity $q(x) \sim Ai(x)$ as $x \to +\infty$. Here $Ai(x)$ denotes the Airy function.

To consider the joint distribution of the largest eigenvalues at the edge of the spectrum, we rescale the eigenvalues as

$$\lambda_j^{(n)} = 2 + \xi_j^{(n)} n^{-2/3}, \quad j = 1, 2, \dots, n, \tag{3}$$

where $\lambda_1^{(n)} \ge \lambda_2^{(n)} \cdots \ge \lambda_n^{(n)}$ are the ordered eigenvalues of A_n. It then follows from the results of [14, 19] that the random point configuration $\{\xi_j^{(n)}, 1 \le j \le n\}$ converges in distribution on the cylinder sets to the random point process on the real line with the k-point correlation functions given by

$$\rho_k(x_1, \dots, x_k) = \big(\det(K(x_i, x_j))_{1\le i,j\le k}\big)^{1/2}, \tag{4}$$

where $K(x, y)$ is a 2×2 matrix-valued kernel with the entries

$$K_{11}(x, y) = K_{Airy}(x, y) + \frac{1}{2}Ai(x)\left(1 - \int_y^{+\infty} Ai(z)dz\right), \tag{5}$$

$$K_{12}(x, y) = -\partial_y K_{Airy}(x, y) - \frac{1}{2}Ai(x)Ai(y), \tag{6}$$

$$K_{21}(x, y) = -\int_x^{+\infty} K_{Airy}(z, y)dz + \frac{1}{2}\left(\int_y^x Ai(z)dz + \int_x^{+\infty} Ai(z)dz \int_y^{+\infty} Ai(z)dz\right), \tag{7}$$

$$K_{22}(x, y) = K_{11}(y, x), \tag{8}$$

and the Airy kernel $K_{Airy}(x, y)$ is defined as

$$K_{Airy}(x, y) = \int_0^{+\infty} Ai(x + z)Ai(y + z)dz = \frac{Ai(x)Ai'(y) - Ai'(x)Ai(y)}{x - y}. \tag{9}$$

Therefore, the k-point correlation function of the limiting random point process is given by the square root of the determinant of the $2k \times 2k$ matrix defined in (4) and (5). One can also rewrite the k-point correlation function in the pfaffian form (see e.g. [9]) which shows that the limiting random point process belongs to the family of the pfaffian random point processes (see e.g. [15]). In particular, the rightmost particle of this pfaffian random point process is given by the Tracy-Widom distribution (2). Moreover, it was shown in [12] that the asymptotic behavior of the largest eigenvalues is universal for Wigner real symmetric matrices with sub-

Gaussian and symmetrically distributed entries. We refer to [10] for recent results on wigner matrices with nonsymmetrically distributed entries.

Define

$$G_n(z) = \left(A_n - 2 - zn^{-2/3}\right)^{-1} \tag{10}$$

for complex z with non-zero imaginary part $\operatorname{Im} z \neq 0$. Here and throughout the paper, we will use $(A_n - z)^{-1}$ as the shorthand notation for the resolvent matrix $(A_n - zId)^{-1}$.

Let

$$\begin{aligned} g_{n,k}(z) &= n^{-2k/3} \operatorname{Tr} G_n^k(z) = n^{-2k/3} \operatorname{Tr}\left(A_n - 2 - zn^{-2/3}\right)^{-k} \\ &= \sum_1^n \left(\xi_j^{(n)} - z\right)^{-k} \end{aligned} \tag{11}$$

for positive integers $k = 1, 2, \ldots$. It can be shown that for $k \geq 2$, $g_{n,k}(z)$ is a "local" statistic of the largest eigenvalues in the GOE. Indeed, only eigenvalues from the $O(n^{-2/3})$-neighborhood of the right edge of the spectrum give non-vanishing contribution to $g_{n,k}(z)$ in the limit $n \to \infty$. For example, the joint contribution of the eigenvalues from $(-\infty, 2 - \delta]$ can be trivially bounded in absolute value by $n^{1-2k/3}|\delta + zn^{-2/3}|^k = o(1)$ for large n uniformly in z with $\operatorname{Re} z$ bounded from below. More delicate estimates involving the asymptotics of the one-point correlation function, imply that the joint contribution of the eigenvalues from $(-\infty, 2-n^{-2/3+\varepsilon})$ to $g_{n,k}(z)$ is still negligible for all $\varepsilon > 0$ and $k > 1$. Moreover, the one-point correlation function $\rho_1(x)$ of the limiting pfaffian random point process defined in (3)–(9) decays super-exponentially at $+\infty$ and grows proportionally to $|x|^{1/2}$ at $-\infty$. Consequently, if $\xi = \{\xi_j,\ j \in \mathbb{Z}\}$ is a random point configuration of the limiting pfaffian random process then

$$\mathbb{E} \sum_j |\xi_j - z|^{-k} = \int_{-\infty}^{+\infty} |x - z|^{-k} \rho_1(x) dx < \infty \tag{12}$$

for any integer $k \geq 2$. The integral at the r.h.s. of (12) diverges for $k = 1$ which emphasizes the fact that $g_{n,1}(z)$ is not a "local statistic" as the main contribution to $g_{n,1}(z) = n^{-2/3} \operatorname{Tr}(A_n - 2 - zn^{-2/3})^{-1}$ comes from the eigenvalues in the bulk. Moreover, it could be shown from the asymptotics of the GOE one-point correlation function that

$$\mathbb{E}\left(\operatorname{Tr}\left(A_n - 2 - zn^{-2/3}\right)^{-1}\right) = -n + O(n^{2/3}). \tag{13}$$

Eventhough the eigenvalues from the bulk of the spectrum give the main contribution to the mathematical expectation of $\operatorname{Tr}(A_n - 2 - zn^{-2/3})^{-1}$, their joint contribution to the fluctuations of $\operatorname{Tr}(A_n - 2 - zn^{-2/3})^{-1}$ around its mean is much smaller (namely, it can be shown to be of order of constant if one smoothes their contribution by a test function with the support inside $[-2 + \delta, 2 - \delta]$). On the other hand, the largest eigenvalues of A_n give smaller (namely, of the order of $O(n^{2/3})$) contribution to the mean of $\operatorname{Tr}(A_n - 2 - zn^{-2/3})^{-1}$ but they give the main contribution to

the fluctuations of $\mathrm{Tr}(A_n - 2 - zn^{-2/3})^{-1}$ around its mean. This suggests to consider

$$g^c_{n,1}(z) = n^{-2/3}\,(n + \mathrm{Tr}\,G_n(z)) = n^{-2/3}\big(n + \mathrm{Tr}\big(A_n - 2 - zn^{-2/3}\big)^{-1}\big) \tag{14}$$

which is a "local" statistic in a sense that the main contribution to $g^c_{n,1}(z)$ comes from the largest eigenvalues (i.e. the eigenvalues that deviate from the right edge of the spectrum on the order of $O(n^{-2/3})$).

In Theorem 1, we obtain the recursive relations on the joint moments of the local linear statistics $g^c_{n,1}(z)$ and $g_{n,k}(z)$, $k \geq 2$. Let K be a multi-index, $K = (k_1, \ldots, k_j)$, $j \geq 1$, with the components k_l, $1 \leq l \leq j$, nonnegative integers. The number of components j is not fixed. We will denote by m_K the corresponding joint moment of $g^c_{n,1}(z)$ and $g_{n,k}(z)$, $k \geq 2$, namely:

$$m_K = \mathbb{E}\left(\big(g^c_{n,1}(z)\big)^{k_1} \prod_{l=2}^{j} (g_{n,l}(z))^{k_l}\right). \tag{15}$$

Let e_l denote the multi-index with the l-th component equal to 1 and the other components equal to zero.

Theorem 1. *Let K be a non-zero multi-index, then the following equation holds*:

$$\begin{aligned} &m_K(z + O(n^{-2/3})) - m_{K+2e_1}(1 + O(n^{-2/3})) - m_{K+e_2}(1 + O(n^{-2/3})) \\ &\quad - 2\sum_{l\geq 1} l k_l m_{K-e_l+e_{l+2}}(1 + O(n^{-2/3})) = O(n^{-1/3}) m_{K+e_1}. \end{aligned} \tag{16}$$

Also, the following "boundary" condition holds:

$$z + O(n^{-2/3}) - m_{2e_1}(1 + O(n^{-2/3})) - m_{e_2}(1 + O(n^{-2/3})) = O(n^{-1/3}) m_{e_1}. \tag{17}$$

Remark 2. We will always assume in (16) that $k_l m_{K-e_l+e_{l+2}} = 0$ if $k_l = 0$. The bounds on the error term in (16) and (17) are uniform for z from compact subsets of $\{z : \mathrm{Im}\, z > 0\}$.

Theorem 1 will be proved in the next section. Let us now consider the Gaussian Unitary Ensemble (GUE) of Hermitian $n \times n$ random matrices.

$$A_n = \frac{1}{\sqrt{n}} (a_{jk})_{j,k=1}^n, \tag{18}$$

where $\{\mathrm{Re}\, a_{jk} = \mathrm{Re}\, a_{kj}\}_{j<k}$ and $\{\mathrm{Im}\, a_{jk} = -\mathrm{Im}\, a_{kj}\}_{j<k}$ are i.i.d. $N(0, 1/2)$ random variables, and $\{a_{ii}\}_{1\leq i\leq n}$ are i.i.d. $N(0, 1)$ random variables.

The global distribution of the eigenvalues of A_n still satisfies the Wigner semicircle law in the limit $n \to \infty$. The limiting local distribution of the largest eigenvalues of A_n was calculated by Tracy and Widom in [16]. In particular,

$$\lim_{n\to\infty} \mathbb{P}\left(\lambda_{\max} \leq 2 + xn^{-2/3}\right) = F_2(x) = \exp\left(-\int_x^\infty (t - x) q^2(t)\, dt\right), \tag{19}$$

where, as before, $q(x)$ is the solution of the Painléve II differential equation with the same asymptotics at infinity.

Consider the same rescaling at the right edge of the spectrum as in the GOE case, namely

$$\lambda_j^{(n)} = 2 + \xi_j^{(n)} n^{-2/3}, \quad j = 1, 2, \dots, \tag{20}$$

where $\lambda_1^{(n)} \geq \lambda_2^{(n)} \cdots \geq \lambda_n^{(n)}$ are the ordered eigenvalues of A_n. It then follows from the results of [16] that the random point configuration $\{\xi_j^{(n)},\ 1 \leq j \leq n\}$ converges in distribution on the cylinder sets to the random point process on the real line with the k-point correlation functions given by

$$\rho_k(x_1, \dots, x_k) = \det\big(K(x_i, x_j)\big)_{1 \leq i, j \leq k} \tag{21}$$

where $K(x, y) = K_{Airy}(x, y)$ is the Airy kernel defined in (9). The limiting random point process belongs to the class of determinantal random point processes (see [13, 6]).

Let us use the same notations $G_n(z)$, $g_{n,k}(z)$, $g^c_{n,1}(z)$, and M_K in the GUE case as they were defined in (10), (11), (14), and (15) in the GOE case above. The following analogue of the Theorem 1 holds:

Theorem 3. *Let K be a non-zero multi-index, then the following equation holds*:

$$\begin{aligned} &m_K(z + O(n^{-2/3})) - m_{K+2e_1}(1 + O(n^{-2/3})) \\ &\quad - \sum_{l \geq 1} l k_l m_{K - e_l + e_{l+2}}(1 + O(n^{-2/3})) = O(n^{-1/3}) m_{K+e_1}. \end{aligned} \tag{22}$$

Also, the following "boundary" condition holds:

$$z + O(n^{-2/3}) - m_{2e_1}(1 + O(n^{-2/3})) = O(n^{-1/3}) m_{e_1}. \tag{23}$$

We now turn our attention to Wishart (a.k.a Laguerre) ensembles of random matrices. Again, we start with the real case. Let $A = A_{n,N} = \frac{1}{\sqrt{n}}(a_{ij})$ be a rectangular $n \times N$ matrix with $\{a_{ij},\ 1 \leq i \leq n,\ 1 \leq j \leq N\}$ real i.i.d. $N(0, 1)$ random variables. Let us assume that $N \geq n$, and $N - n = \nu$ is fixed. Consider a nonnegative-definite random matrix

$$M_{n,N} = AA^t. \tag{24}$$

The ensemble of random matrices $M_{n,N}$ is known as the real Wishart distribution in the statistical literature or the Laguerre ensemble in the mathematical physics. The empirical distribution function of the eigenvalues of $M_{n,N}$ converges to the Marchenko-Pastur law as $n \to \infty$ [8, 11]. The density of the Marchenko-Pastur law is given by

$$\rho_{\mathrm{MP}}(x) = \begin{cases} \frac{1}{2\pi\sqrt{x}}\sqrt{4 - x} & \text{if } 0 \leq x \leq 4, \\ 0 & \text{otherwise.} \end{cases} \tag{25}$$

Our goal is to study the distribution of the smallest eigenvalues of $M_{n,N}$ in the limit $n \to \infty$, $N - n = \nu$. It can be shown (see e.g. [4, 5, 3]) that the smallest

eigenvalue of $M_{n,N}$ are of the order of n^{-2}. Moreover, if we consider the rescaling at the hard edge of the spectrum

$$\lambda_i^{(n,N)} = \frac{\xi_i^{(n,N)}}{4n^2}, \quad 1 \le i \le n, \tag{26}$$

one can show that the random point configuration $\{\xi_i^{(n)},\ 1 \le i \le n\}$ converges in distribution on the cylinder sets to the pfaffian random point process on $(0, +\infty)$. The k-point correlation functions of the limiting process are of the same form as in (4), where $K(x, y)$ is again a 2×2 matrix-valued kernel. The formulas for the entries of $K(x, y)$ are similar to (5) with the important difference being that the Airy kernel $K_{Airy}(x, y)$ is replaced by the Bessel kernel

$$K_{Bessel}(x, y) = \frac{J_\nu(\sqrt{x})\sqrt{y}J_{\nu+1}(\sqrt{y}) - J_\nu(\sqrt{y})\sqrt{x}J_{\nu+1}(\sqrt{x})}{2(x-y)}, \tag{27}$$

where $J_\nu(x)$ is the usual Bessel function of index ν.

Define

$$G_{n,N}(t) = \left(M_{n,N} + \frac{t^2}{n^2}\right)^{-1}, \tag{28}$$

where t is a real number. Then

$$\begin{aligned} g_k(t) = g_{n,N,k}(t) &= n^{-2k}\,\mathrm{Tr}\,G_{n,N}^k(t) = n^{-2k}\,\mathrm{Tr}\left(M_{n,N} + \frac{t^2}{n^2}\right)^{-k} \\ &= \sum_1^n \left(\xi_i^{(n,N)} + t^2\right)^{-k} \end{aligned} \tag{29}$$

is a "local" statistics for any positive integer $k = 1, 2, 3, \ldots$. Indeed, one can show that the eigenvalues from the bulk of the spectrum give vanishing contribution to $g_k(t)$. In particular, if $\xi = \{\xi_i,\ i \in \mathbb{N}\}$ is a random point configuration of the limiting pfaffian process, then

$$\mathbb{E}\sum_j (\xi_j + t^2)^{-k} = \int_0^{+\infty} \frac{1}{(x+t^2)^k}\rho_1(x)dx < \infty. \tag{30}$$

We are interested to study the joint moments of the linear statistics $g_k(t)$, $k \ge 1$. Let, as before, $K = (k_1, \ldots, k_j)$, $j \ge 1$, denote a multi-index, and m_K stand for the corresponding joint moment

$$m_K = \mathbb{E}\prod_{l=1}^{j} (g_l(t))^{k_l}. \tag{31}$$

The following theorem holds.

Theorem 4. *Let K be a non-zero multi-index, then the following equation holds*:

$$\left(\nu - t^{-2} + \frac{1}{n}\right) m_{K+e_1} + m_{K+e_2} + m_{K+2e_1} + 2\sum_{l=1}^{j} l k_l m_{K-e_l+e_{l+2}}$$
$$- \frac{2}{t^2}\sum_{l=1}^{j} l k_l m_{K-e_l+e_{l+1}}$$
$$= \frac{1}{n}\frac{1}{t^2} m_K. \tag{32}$$

Also, the following "boundary" condition holds:

$$\left(\nu - t^{-2} + \frac{1}{n}\right) m_{e_1} + m_{e_2} + m_{2e_1} = t^{-2}. \tag{33}$$

We recall that $\nu = N - n \geq 0$ is the difference between the dimensions of the rectangular matrix $A_{n,N}$.

We finish the Introduction by the discussion of the complex Wishart ensemble. Let $A = A_{n,N} = \frac{1}{\sqrt{n}}(a_{ij})$ be a rectangular $n \times N$ matrix with $\{\mathrm{Re}\, a_{ij}, \mathrm{Im}\, a_{ij},\ 1 \leq i \leq n,\ 1 \leq j \leq N,\}$ i.i.d. $N(0, 1/2)$ random variables. As before, we us assume that $N \geq n$, and $N - n = \nu$ is fixed. Consider now a nonnegative-definite random matrix

$$M_{n,N} = AA^*. \tag{34}$$

The ensemble of random matrices $M_{n,N}$ is known as the complex Wishart/Laguerre ensemble of random matrices. Consider the rescaling of the eigenvalues at the hard edge of the spectrum

$$\lambda_i^{(n,N)} = \frac{\xi_i^{(n,N)}}{4n^2}, \quad 1 \leq i \leq n. \tag{35}$$

It follows from the results of [4, 17] that the random point configuration $\{\xi_i^{(n)}, i \geq 1\}$ converges in distribution on the cylinder sets to the determinantal random point process on $(0, +\infty)$ with the correlation kernel given by the Bessel kernel (27) in the limit $n \to \infty$, $N = n + \nu$. For universality results, we refer to [2]. Define $G_{n,N}$, $g_k(t)$, $k \geq 1$, and m_K in the same way as in (28), (29), and (31). The following theorem holds.

Theorem 5. *Let K be a non-zero multi-index, then the following equation holds:*

$$\left(\nu + \frac{1}{n}\right) m_{K+e_1} + m_{K+2e_1} + \sum_{l=1}^{j} l k_l m_{K-e_l+e_{l+2}} - \frac{1}{t^2}\sum_{l=1}^{j} l k_l m_{K-e_l+e_{l+1}}$$
$$= \frac{1}{n}\frac{1}{t^2} m_K. \tag{36}$$

Also, the following "boundary" condition holds:

$$\left(\nu + \frac{1}{n}\right) m_{e_1} + m_{2e_1} = t^{-2}. \tag{37}$$

We recall that $v = N - n \geq 0$ is the difference between the dimensions of the rectangular matrix $A_{n,N}$. Theorems 4 and 5 will be proved in Sect. 3.

2 Proof of Theorems 1 and 3

Let us start with the proof of Theorem 1. Our first goal is to establish (17). To this end, we consider $n^{1/3}m_{e_1} = \mathbb{E}(n^{-1/3}(n + \operatorname{Tr} G_n(z)))$, where, as before, $G_n(z) = (A_n - 2 - zn^{-2/3})^{-1}$. By using the resolvent identity

$$\begin{aligned} G_n(z) &= \big(A_n - 2 - zn^{-2/3}\big)^{-1} \\ &= -\big(2 + zn^{-2/3}\big)^{-1} Id + \big(2 + zn^{-2/3}\big)^{-1} A_n \big(A_n - 2 - zn^{-2/3}\big)^{-1} \\ &= -\big(2 + zn^{-2/3}\big)^{-1} Id + \big(2 + zn^{-2/3}\big)^{-1} A_n G_n, \end{aligned} \tag{38}$$

we arrive at

$$n^{1/3}m_{e_1} = n^{2/3} - \big(2 + zn^{-2/3}\big)^{-1} n^{2/3} + \big(2 + zn^{-2/3}\big)^{-1} n^{-1/3} \mathbb{E} \sum_{ij} A_{ij} G_{ji}. \tag{39}$$

Here $A_{ij} = \frac{a_{ij}}{\sqrt{n}}$ denote the matrix entries of A_n, and G_{ij} denote the matrix entries of $G_n(z)$. To calculate $\mathbb{E}A_{ij}G_{ji}$, we recall that random variables A_{ij}, $1 \leq i \leq j \leq n$, are independent. Therefore, we can first fix all matrix entries (up from the diagonal) except A_{ij} and integrate with respect to A_{ij}. Applying the Gaussian decoupling formula

$$\mathbb{E}\eta f(\eta) = \sigma^2 \mathbb{E} f'(\eta), \eta \sim N(0, \sigma^2), \tag{40}$$

with $\eta = A_{ij}$ and $f(\eta) = G_{ij}$, and taking into account that $\operatorname{Var}(A_{ij}) = \frac{1+\delta_{ij}}{n}$, and

$$\frac{\partial G_{kl}}{\partial A_{ij}} = \begin{cases} -G_{ki}G_{jl} - G_{kj}G_{il} & i \neq j, \\ -G_{ki}G_{jl} & i = j, \end{cases} \tag{41}$$

we arrive at

$$\begin{aligned} n^{1/3}m_{e_1} = n^{2/3} &- \big(2 + zn^{-2/3}\big)^{-1} n^{2/3} \\ &- \big(2 + zn^{-2/3}\big)^{-1} n^{-4/3} \mathbb{E} \sum_{ij} (G_{ji}G_{ji} + G_{ii}G_{jj}). \end{aligned} \tag{42}$$

The term $n^{-4/3}\mathbb{E}\sum_{ij} G_{ji}G_{ji}$ is equal to

$$n^{-4/3}\mathbb{E} \sum_{ij} G_{ji}G_{ji} = \mathbb{E}n^{-4/3} \operatorname{Tr}\big(G_n^2(z)\big) = m_{e_2}. \tag{43}$$

To deal with the term $n^{-4/3}\mathbb{E}\sum_{ij} G_{ii}G_{jj}$, we rewrite it as

$$
\begin{aligned}
n^{-4/3}\mathbb{E}\sum_{ij} G_{ii}G_{jj} &= n^{-4/3}\mathbb{E}\big((\operatorname{Tr} G_n(z))^2\big) \\
&= n^{-4/3}\mathbb{E}\big((-n+n+\operatorname{Tr} G_n(z))^2\big) \\
&= n^{2/3} - 2n^{-1/3}\mathbb{E}(n+\operatorname{Tr} G_n(z)) + n^{-4/3}\mathbb{E}\big((n+\operatorname{Tr} G_n(z))^2\big) \\
&= n^{2/3} - 2n^{1/3}m_{e_1} + m_{2e_1}. \qquad (44)
\end{aligned}
$$

As a result, we obtain

$$
\begin{aligned}
n^{1/3}m_{e_1} = n^{2/3} &- (2+zn^{-2/3})^{-1}n^{2/3} - (2+zn^{-2/3})^{-1}m_{e_2} \\
&- (2+zn^{-2/3})^{-1}n^{2/3} + 2(2+zn^{-2/3})^{-1}n^{1/3}m_{e_1} \\
&- (2+zn^{-2/3})^{-1}m_{2e_1}, \qquad (45)
\end{aligned}
$$

which is equivalent to

$$
\begin{aligned}
&n^{2/3}(1-(1+zn^{-2/3}/2)^{-1}) - m_{2e_1}(2+zn^{-2/3})^{-1} - m_{e_2}(2+zn^{-2/3})^{-1} \\
&\quad = m_{e_1}n^{1/3}(1-(1+zn^{-2/3}/2)^{-1}). \qquad (46)
\end{aligned}
$$

After trivial arithmetical simplifications, this leads to (17). The formula (16) can be proven along the same lines if one starts with $n^{1/3}m_{K+e_1}$. One can say that the formula (17) gives us the boundary term in the recursive system of linear equations satisfied by $\{m_K\}$ since it corresponds to $K=0$. Turning our attention to (16), we write

$$
\begin{aligned}
n^{1/3}m_{K+e_1} &= n^{1/3}\mathbb{E}\left((g^c_{n,1}(z))^{k_1+1}\prod_{l=2}^{j}(g_{n,k}(z))^{k_l}\right) \\
&= \mathbb{E}\Big[n^{-1/3}(n+\operatorname{Tr} G_n)\big(n^{-2/3}(n+\operatorname{Tr} G_n)\big)^{k_1}\prod_{l\geq 2}\big(n^{-2l/3}\operatorname{Tr} G^l\big)^{k_l}\Big], \qquad (47)
\end{aligned}
$$

we then rewrite, as before, the first term $n^{-1/3}(n+\operatorname{Tr} G_n)$ as

$$
n^{-1/3}(n+\operatorname{Tr} G_n) = n^{2/3} - (2+zn^{-2/3})^{-1}n^{2/3} + (2+zn^{-2/3})^{-1}n^{-1/3}\sum_{ij} A_{ij}G_{ji}. \qquad (48)
$$

This leads to

$$
\begin{aligned}
n^{1/3}m_{K+e_1} &= n^{2/3}m_K - (2+zn^{-2/3})^{-1}n^{2/3}m_K \\
&\quad + (2+zn^{-2/3})^{-1}n^{-1/3} \\
&\quad \times \mathbb{E}\left[\left(\sum_{ij} A_{ij}G_{ji}\right)\big(n^{-2/3}(n+\operatorname{Tr} G_n)\big)^{k_1}\prod_{l\geq 2}\big(n^{-2l/3}\operatorname{Tr} G^l\big)^{k_l}\right]. \qquad (49)
\end{aligned}
$$

As in the case $K = 0$ considered above, we fix all matrix entries (up from the diagonal) except A_{ij}, and apply (40) with $\eta = A_{ij}$ and $f(\eta) = G_{ji}(n^{-2/3}(n + \operatorname{Tr} G_n))^{k_1} \prod_{l\geq 2}(n^{-2l/3} \operatorname{Tr} G^l)^{k_l}$. Taking into account (41) and the equation

$$\frac{\partial \operatorname{Tr}(G^l)}{\partial A_{ij}} = -2l(G^{l+1})_{ij}, \tag{50}$$

one then obtains (16) after some simple algebraic calculations. Theorem 1 is proven.

The proof of Theorem 3 is quite similar. The only alteration required in the GUE case is that one needs to replace (41) with

$$\frac{\partial G_{kl}}{\partial Re(A_{ij})} = \begin{cases} -G_{ki}G_{jl} - G_{kj}G_{il} & i \neq j \\ -G_{ki}G_{jl} & i = j, \end{cases} \tag{51}$$

and

$$\frac{\partial G_{kl}}{\partial Im(A_{ij})} = -i(G_{ki}G_{jl} - G_{kj}G_{il}) \quad \text{for } i \neq j. \tag{52}$$

The remaining calculations are very similar and are left to the reader.

3 Proof of Theorems 4 and 5

The proofs will be similar to the ones given in the previous section. Let us start with the proof of Theorem 4. Our first goal is to establish (33). To this end, we consider $n^{-1}m_{e_1} = \mathbb{E}(n^{-3} \operatorname{Tr} G_{n,N}(t))$, where $G_{n,N}(t)$ was defined in (28). By using the resolvent identity

$$G_{n,N} = \left(M_{n,N} + \frac{t^2}{n^2}\right)^{-1} = \frac{n^2}{t^2}Id - \frac{n^2}{t^2}AA^tG_{n,N} \tag{53}$$

we arrive at

$$n^{-1}m_{e_1} = \frac{1}{t^2} - \frac{1}{n}\frac{1}{t^2}\mathbb{E}\sum_{1\leq i,j\leq n}\sum_{1\leq p\leq N} A_{ip}A_{jp}G_{ji}. \tag{54}$$

Here $A_{ip} = \frac{a_{ip}}{\sqrt{n}}$ denote the matrix entries of A_n, and G_{ji} denote the matrix entries of $G_{n,N}(z)$. To calculate $\mathbb{E}A_{ip}A_{jp}G_{ji}$, we again use the Gaussian decoupling formula (40) and the equation

$$\frac{\partial G_{kl}}{\partial A_{ip}} = -G_{ki}(A^tG)_{pl} - (GA)_{kp}G_{il}. \tag{55}$$

Therefore,

$$n^{-1}m_{e_1} = \frac{1}{t^2} + \frac{1}{n^2}\frac{1}{t^2}\mathbb{E}\sum_{1\le i,j\le n}\sum_{1\le p\le N} A_{jp}\left(G_{ji}(GA)_{ip} + G_{ii}(GA)_{jp}\right)$$
$$- \frac{1}{n^2}\frac{1}{t^2}\mathbb{E}\sum_{1\le i\le n}\sum_{1\le p\le N} G_{ii}$$
$$= \frac{1}{t^2} + \frac{1}{n^2}\frac{1}{t^2}\mathbb{E}\left[\mathrm{Tr}(GAA^tG) + \mathrm{Tr}(GAA^t)\,\mathrm{Tr}\,G\right] - \frac{N}{n^2}\frac{1}{t^2}\mathbb{E}\,\mathrm{Tr}\,G. \quad (56)$$

Using the identity $GAA^t = Id - \frac{t^2}{n^2}G$, the last formula can rewritten as

$$n^{-1}m_{e_1} = \frac{1}{t^2} + \frac{1}{t^2}m_{e_1} - m_{e_2} + \frac{n}{t^2}m_{e_1} - m_{2e_1} - \frac{n+\nu}{t^2}m_{e_1}, \quad (57)$$

which implies (33). The formula (32) can be proven along the same lines if one starts with $n^{-1}m_{K+e_1}$. Let us write

$$n^{-1}m_{K+e_1} = n^{-1}\mathbb{E}\left((g_1(t))\prod_{l=1}^{j}(g_l(t))^{k_l}\right)$$
$$= \mathbb{E}\left[n^{-3}\,\mathrm{Tr}\,G_{n,N})\prod_{l\ge 1}\left(n^{-2l}\,\mathrm{Tr}\,G_{n,N}^l\right)^{k_l}\right], \quad (58)$$

Using the resolvent identity, we can rewrite the first term in the product as

$$G_{n,N} = \frac{n^2}{t^2}Id - \frac{n^2}{t^2}AA^tG_{n,N}.$$

After integration by parts and a few lines of careful calculations, we obtain (32). Theorem 5 can be proven along similar lines.

4 Non-Gaussian Case

The generalization of the Gaussian decoupling formula (40) to the non-Gaussian case can be found, for example, in [7]:

$$\mathbb{E}[\xi f(\xi)] = \sum_{k=0}^{p}\frac{c_{k+1}}{k!}\mathbb{E}\left[\frac{d^k f}{dx^k}(\xi)\right] + \varepsilon, \quad (59)$$

where ξ is a real random variable such that $\mathbb{E}(|\xi|^{p+2}) < \infty$, $c_l, l \ge 1$, are the cumulants of the random variable ξ, complex-valued function $f(x)$ has first $p+1$ continuous and bounded derivatives, and the error term satisfies the upper bound $|\varepsilon| \le B_{p+1}sup_x|\frac{d^{p+1}f}{dx^{p+1}}(x)|\mathbb{E}(|\xi|^{p+2})$ with the constant B_{p+1} depending only on $p+1$.

It is conjectured that the distribution of the largest eigenvalues in Wigner random matrices is universal provided the fourth moment of the matrix entries is finite. Currently, we are unable to prove this conjecture. Instead, we speculate below on the possible approach to extend the results of Theorems 1, 3–5 to the non-Gaussian case. Let us consider a real Wigner random matrix $A_n = \frac{1}{\sqrt{n}}(a_{ij})_{i,j=1}^n$, and assume that the entries $(a_{ij} = a_{ji})_{i<j}$ are i.i.d. centralized random variables with the unit variance and the finite fourth moment. In addition, we assume that the diagonal entries a_{ii}, $1 \le i \le n$, are i.i.d. centralized random variables, independent from the non-diagonal entries. We assume that the diagonal entries also have the finite fourth moment. Let us also assume for simplicity that $\mathrm{Var}(a_{ii}) = 2$. In an attempt to extend the result of Theorem 1 to the non-Gaussian situation, we apply the generalized decoupling formula (59). To be specific, let us concentrate our attention on the "boundary" equation (17). Looking at (39), we apply (59) to $\mathbb{E}A_{ij}G_{ji}$. Since $c_1(a_{ij}) = 0$, $c_2(a_{ij}) = 1 + \delta_{ij}$, $c_3(a_{ij}) = c_3$, for $i < j$, and $\mathbb{E}a_{ij}^4 \le \infty$, one might wish to truncate (59) after the first three terms (i.e. $p = 2$) to obtain

$$n^{-1/3}\mathbb{E}\sum_{ij} A_{ij}G_{ji} = -n^{-4/3}\mathbb{E}\sum_{ij}\left(G_{ji}^2 + G_{ii}G_{jj}\right) + n^{-11/6}\mathbb{E}\sum_{ij}\left(3G_{ij}G_{ii}G_{jj} + G_{ij}^3\right) + \epsilon. \tag{60}$$

The first sum in (60) is the same as in the Gaussian case. The hope is to show that the second sum and the remainder term give negligible contributions in the limit $n \to \infty$. However, it is currently unclear to us how to efficiently bound the terms $n^{-11/6}\mathbb{E}\sum_{ij} G_{ij}G_{ii}G_{jj}$ and $n^{-11/6}\mathbb{E}\sum_{ij} G_{ij}^3$.

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Energy Current Correlations for Weakly Anharmonic Lattices

Herbert Spohn

Abstract We discuss properties of the Boltzmann-Peierls equation for weakly anharmonic lattice dynamics. In particular, we explain how energy type correlations are predicted from this transport equation. An intriguing application is the famous Fermi-Pasta-Ulam β chain, for which we prove that the energy current correlations in equilibrium decay for long times as $t^{-3/5}$, in the kinetic approximation.

1 Introduction

A solid transports energy. Besides the mobile electrons, one important mechanism for energy transport are the vibrations of the crystal lattice. There is no difficulty in writing down the appropriate lattice dynamics. To extract from it the thermal conductivity remains a fairly untractable problem. The most successful approach exploits that even rather close to the melting temperature the typical deviations of the crystal atoms from their equilibrium position are small as compared to the lattice constant. This observation then leads to the phonon kinetic equation, which goes back to the seminal paper by Peierls [9]. (For electron transport a corresponding idea was put forward by Nordheim [6].) Phonon kinetic theory flourished in the 50ies, an excellent account of the 1960 status being the book by Ziman [17]. Of course, transport of heat and thermal conductivity remain an important experimental research area, in particular since novel materials become available and since more extreme properties are in demand. On the other hand, if the very recent collection of articles by Tritt [15] is taken to be representative, it is obvious that after 1960 hardly any new elements have been added to the theory. The real innovation are fast and efficient molecular dynamics algorithms. The currently available techniques allow the simulation of $6 \times 6 \times 6$ periodized lattices with two atoms per unit cell [5].

Herbert Spohn
Zentrum Mathematik and Physik Department, TU München, Boltzmannstr. 3, 85747 Garching, Germany, e-mail: spohn@ma.tum.de

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According to the Green-Kubo formula the thermal conductivity is determined through the time-integral over the energy current correlation in thermal equilibrium. In my contribution I will explain its structure for weakly anharmonic lattices. While I do not add anything novel in substance, I believe that, with the post 1960 insights gained from the kinetic theory of rarified gases, the story can be presented more concisely and systematically than done usually. As a bonus, the mathematical physics issues left unresolved will become more sharply in focus.

2 Anharmonic Lattice Dynamics

Physically, one starts from a given crystal structure, which means to specify the lattice and the number of atoms per unit cell. The interaction potential is expanded in the displacements away from the equilibrium positions. Then the first order term vanishes, because one expands at a stationary point. The second order term is the harmonic approximation and higher order terms are regarded as small corrections. It is argued that for real crystals mostly the third order term suffices unless there are special symmetries which make it vanish and requires to go to fourth order. In this article, the focus will be on the analysis of the linearized Boltzmann equation and its relation to the energy current correlations. For this purpose we take the liberty to employ a single band model for the anharmonic lattice dynamics. There is no difficulty, in principle, to add on extra features so to make the model more realistic.

We assume a simple hypercubic lattice $\mathbb{Z}^d$ with a single atom per unit cell. Physically $d = 3$, but we keep the general dimension d because of recent interest in chains, for which $d = 1$. A single band model corresponds to scalar atomic displacements.

Fourier transform will be convenient. Let $\mathbb{T}^d = [-\frac{1}{2}, \frac{1}{2}]^d$ be the first Brioullin zone of the dual lattice. For $f : \mathbb{Z}^d \to \mathbb{R}$ its Fourier transform, $\widehat{f}$, is defined by

$$\widehat{f}(k) = \sum_{x \in \mathbb{Z}^d} e^{-i2\pi k \cdot x} f_x. \tag{1}$$

Here $k \in \mathbb{T}^d$ and $\widehat{f}(k)$ extends periodically to a function on $\mathbb{R}^d$. The inverse Fourier transform is given by

$$f_x = \int_{\mathbb{T}^d} dk e^{i2\pi k \cdot x} \widehat{f}(k). \tag{2}$$

For $x \in \mathbb{Z}^d$ the deviation away from x is denoted by $q_x \in \mathbb{R}$. The corresponding momentum is denoted by $p_x \in \mathbb{R}$. We choose units such that the atomic mass equals one. The harmonic approximation to the interaction potential reads

$$U_{\text{harm}}(q) = \frac{1}{2} \sum_{x,y \in \mathbb{Z}^d} \alpha(x - y) q_x q_y. \tag{3}$$

The elastic constants $\alpha(x)$ satisfy

$$\alpha(x) = \alpha(-x), \quad |\alpha(x)| \leq \gamma_0 e^{-\gamma_1|x|} \tag{4}$$

for suitable constants $\gamma_0, \gamma_1 > 0$. Mechanical stability requires

$$\widehat{\alpha}(k) \geq 0. \tag{5}$$

In addition, because of the invariance of the interaction between crystals atoms under the translation $q_x \rightsquigarrow q_x + a$, one imposes

$$\sum_{x\in\mathbb{Z}^d} \alpha(x) = 0, \quad \text{i.e. } \widehat{\alpha}(0) = 0. \tag{6}$$

For an optical band, because of the internal structure of the unit cell, the condition (6) is not satisfied, which in the framework of our model can be interpreted as adding to the physical harmonic interaction satisfying (6) a harmonic on-site potential of the form

$$U_{\text{site}}(q) = \frac{1}{2}\omega_0^2 \sum_{x\in\mathbb{Z}^d} q_x^2. \tag{7}$$

The harmonic lattice dynamics is governed by the Hamiltonian

$$H_{\text{ha}} = \frac{1}{2}\sum_{x\in\mathbb{Z}^d}(p_x^2 + \omega_0^2 q_x^2) + \frac{1}{2}\sum_{x,y\in\mathbb{Z}^d} \alpha(x-y) q_x q_y \tag{8}$$

and has plane wave solutions with dispersion relation

$$\omega(k) = (\omega_0^2 + \widehat{\alpha}(k))^{1/2}. \tag{9}$$

Clearly, $\omega(k) = \omega(-k)$ and $\omega(k) \geq \omega_0 \geq 0$. We concatenate q_x and p_x into a single complex-valued field $a(k)$ as

$$a(k) = \frac{1}{\sqrt{2}}\left(\sqrt{\omega(k)}\widehat{q}(k) + i\frac{1}{\sqrt{\omega(k)}}\widehat{p}(k)\right) \tag{10}$$

with the inverse

$$\begin{aligned} \widehat{q}(k) &= \frac{1}{\sqrt{2}}\frac{1}{\sqrt{\omega(k)}}\big(a(k) + a(-k)^*\big), \\ \widehat{p}(k) &= \frac{i}{\sqrt{2}}\sqrt{\omega(k)}\big(-a(k) + a(-k)^*\big). \end{aligned} \tag{11}$$

The a-field evolves as

$$\frac{\partial}{\partial t}a(k,t) = -i\omega(k)a(k,t). \tag{12}$$

In nature lattice vibrations are quantized. In our model this is easily implemented by promoting $a(k)^*$ and $a(k)$ to creation and annihilation operators of a scalar Bose field. $a(k)^*$ is the operator adjoint to $a(k)$ and the $a(k)$'s satisfy the canonical com-

mutation relations

$$[a(k), a(k')^*] = \delta(k - k'), \qquad [a(k), a(k')] = 0. \tag{13}$$

The Heisenberg evolution for the a-field is still governed by (12).

Continuing the expansion scheme we add to H_0 the next order terms. The simplest one would be a cubic on-site potential as

$$V_3 = \frac{1}{3} \sum_{x \in \mathbb{Z}^d} q_x^3, \tag{14}$$

which in terms of the a-field reads

$$V_3 = \frac{1}{3} \int_{\mathbb{T}^{3d}} dk_1 dk_2 dk_3 \delta(k_1 + k_2 + k_3) \prod_{j=1}^{3} (2\omega(k_j))^{-1/2} (a(k_j) + a(-k_j)^*). \tag{15}$$

Correspondingly, at fourth order,

$$V_4 = \frac{1}{4} \sum_{x \in \mathbb{Z}^d} q_x^4 \tag{16}$$

which in terms of the a-field becomes

$$\begin{aligned} V_4 = \frac{1}{4} \int_{\mathbb{T}^{4d}} dk_1 dk_2 dk_3 dk_4 \delta(k_1 + k_2 + k_3 + k_4) \\ \times \prod_{j=1}^{4} (2\omega(k_j))^{-1/2} \big(a(k_j) + a(-k_j)^*\big). \end{aligned} \tag{17}$$

$H_{\mathrm{ha}} + \lambda V_3$ is not bounded from below. This can be remedied by adding $\lambda^2 V_4$, for example, which would then not contribute on the kinetic scale.

If the potential depends only on the displacement differences, then the lowest order nonlinearity is

$$V_{3\mathrm{di}} = \frac{1}{3} \sum_{x,y \in \mathbb{Z}^d} \alpha_3(x - y)(q_x - q_y)^3 \tag{18}$$

with $\alpha_3(-x) = -\alpha_3(x)$ and $|\alpha_3|$ exponentially bounded. Switching to the a-field $V_{3\mathrm{di}}$ becomes

$$\begin{aligned} V_{3\mathrm{di}} = \frac{1}{3} \int_{\mathbb{T}^{4d}} dk_1 dk_2 dk_3 \delta(k_1 + k_2 + k_3) \\ \times \sum_{x \in \mathbb{Z}^d} \alpha_3(x) \prod_{j=1}^{3} (2\omega(k_j))^{-1/2} (e^{i2\pi k_j \cdot x} - 1) \big(a(k_j) + a(-k_j)^*\big). \end{aligned} \tag{19}$$

In the kinetic limit the square of the vertex function determines the collision rate. Thus, from the collision rate

$$\prod_{j=1}^{3}(2\omega(k_j))^{-1} \tag{20}$$

for the on-site V_3 the collision rate for $V_{3\mathrm{di}}$ is obtained by the replacement

$$\prod_{j=1}^{3}(2\omega(k_j))^{-1}\left|\sum_{x\in\mathbb{Z}^d}\alpha_3(x)\prod_{j=1}^{3}(e^{i2\pi k_j\cdot x}-1)\right|^2. \tag{21}$$

Because of such a simple substitution rule we continue to work with V_3. The corresponding rule also applies to the switch from V_4 to $V_{4\mathrm{di}}$.

From other areas of mathematical physics one is accustomed to have a given starting Hamiltonian. In our context this means to specify the elastic constants $\alpha(x)$, $\alpha_3(x)$, $\alpha_4(x)$. For real crystals their determination requires a lot of experimental (and also theoretical) efforts, as discussed in [15], see also [16, 8, 7] for a modeling of aluminium and silicon. It would be thus of importance to have a stability result available, which ensures that certain qualitative properties do not depend so much on the specific choice of elastic constants.

3 Energy Current Correlations

Let us consider the Hamiltonian

$$H = H_{\mathrm{ha}} + \lambda V_3 + \lambda^2 V_4. \tag{22}$$

The total energy current correlation function is computed in thermal equilibrium at inverse temperature β. It is denoted by $C_\lambda(t)$ and will be defined below. Since $\lambda \ll 1$, the plan is to compute $C_\lambda(t)$ in the limit of $\lambda \to 0$. The phonons then hardly interact and $C_\lambda(t)$ decays slowly on the time scale λ^{-2}. Thus one expects that the limit

$$\lim_{\lambda\to 0} C_\lambda(\lambda^{-2}t) = C_{\mathrm{kin}}(t) \tag{23}$$

exists and is determined by the phonon Boltzmann equation linearized at equilibrium.

Let us first find the local energy current. Since H is not local, there is some arbitrariness involved in defining the local energy. One conventional choice for the energy at site x is to set

$$H_x = \frac{1}{2}p_x^2 + \frac{1}{2}\omega_0^2 q_x^2 + \frac{1}{2}\sum_{y\in\mathbb{Z}^d}\alpha(x-y)q_x q_y + \frac{1}{3}\lambda q_x^3 + \frac{1}{4}\lambda^2 q_x^4. \tag{24}$$

In the Heisenberg picture H_x becomes time-dependent. Writing $dH_x(t)/dt$ as a divergence, the energy current can be identified with

$$J_x = \frac{1}{4} \sum_{y \in \mathbb{Z}^d} y\alpha(y)(-q_x p_{x+y} + q_{x+y} p_x) \tag{25}$$

which happens to be independent of λ. To verify (25), one chooses a large box Λ with faces $\partial\Lambda$. The energy inside Λ is

$$H_\Lambda(t) = \sum_{x \in \Lambda} H_x(t) \tag{26}$$

and it satisfies

$$\frac{d}{dt} H_\Lambda(t) = -\sum_{x \in \Lambda} n_x \cdot J_x(t) + \mathscr{O}(\partial\Lambda), \tag{27}$$

where n_x is the outward normal to Λ at $x \in \partial\Lambda$. The errors come from the corners of Λ and from the possibly infinite range of α.

With this input the total energy current correlation is defined by

$$\ell \cdot C_\lambda(t)\ell = \sum_{x \in \mathbb{Z}^d} \langle (\ell \cdot J_0(t))(\ell \cdot J_x(0)) \rangle_\beta, \tag{28}$$

where $\ell \in \mathbb{R}^d$, $J_x \in \mathbb{R}^d$, "$\cdot$" is the scalar product in $\mathbb{R}^d$, and $C_\lambda(t)$ is a $d \times d$ matrix. $\langle \cdot \rangle_\beta$ refers to the thermal average with respect to $Z^{-1} e^{-\beta H}$. By time-stationary and time-reversal, $C_\lambda(t)$ is symmetric and it suffices to consider its numerical range. At the expense of an error of order λ, we may replace in $e^{-\beta H}$ the full Hamiltonian H by the harmonic approximation

$$H_{\mathrm{ha}} = \int_{\mathbb{T}^d} dk \omega(k) a(k)^* a(k). \tag{29}$$

For the total current one finds

$$J = \sum_{x \in \mathbb{Z}^d} J_x = \frac{1}{2\pi} \int_{\mathbb{T}^d} dk (\nabla\omega(k)) \omega(k) a(k)^* a(k), \tag{30}$$

where it is used that $\nabla\widehat{\alpha} = 2\omega(\nabla\omega)$. Since $[H_{\mathrm{ha}}, J] = 0$, $\sum_{x \in \mathbb{Z}^d} \ell \cdot J_x$ can be lifted to the exponent. Thus we define the new average $\langle \cdot \rangle_{\beta,\tau}$ with respect to the state $Z^{-1} \exp[-\beta H_{\mathrm{ha}} + \tau \ell \cdot J]$. Then

$$\ell \cdot C_\lambda(t)\ell = \lim_{\tau \to 0} \frac{1}{\tau} \langle \ell \cdot J_0(t) \rangle_{\beta,\tau} + \mathscr{O}(\lambda). \tag{31}$$

The anharmonicity now resides only in the dynamics.

The limit $\lambda \to 0$ on the right hand side in (31) is discussed in [13]. The initial state is spatially homogeneous and determines the Wigner function $W_{\beta,\tau}(k)$ through

$$\langle a(k')^* a(k)\rangle_{\beta,\tau} = \delta(k-k')W_{\beta,\tau}(k) \tag{32}$$

with

$$W_{\beta,\tau}(k) = \big(\exp\big[\beta\omega(k) - \tau(\ell\cdot\nabla\omega(k))\omega(k)\big] - 1\big)^{-1}. \tag{33}$$

On the kinetic time scale, $\lambda^{-2}t$, the Wigner function $W_{\beta,\tau}$ evolves to $W_\tau(t)$ which is determined as the solution of the spatially homogeneous Boltzmann equation. For our model, i.e. for the anharmonic on-site potential V_3, it reads

$$\frac{\partial}{\partial t}W(t) = \mathscr{C}(W(t)) \tag{34}$$

with the collision operator

$$\begin{aligned}\mathscr{C}(W)_1 = \frac{\pi}{2}\int_{\mathbb{T}^{2d}} dk_2dk_3(\omega_1\omega_2\omega_3)^{-1}\\ \times\{2\delta(\omega_1+\omega_2-\omega_3)\delta(k_1+k_2-k_3)(\tilde W_1\tilde W_2W_3 - W_1W_2\tilde W_3)\\ +\delta(\omega_1-\omega_2-\omega_3)\delta(k_1-k_2-k_3)(\tilde W_1W_2W_3 - W_1\tilde W_2\tilde W_3)\}.\end{aligned} \tag{35}$$

Here we use the shorthands $W_j = W(k_j)$, $\omega_j = \omega(k_j)$, $j = 1,2,3$, and $\tilde W(k) = 1 + W(k)$. Using (30), the average in (31) becomes then

$$\langle \ell\cdot J_0(\lambda^{-2}t)\rangle_{\beta,\tau} = \frac{1}{2\pi}\int_{\mathbb{T}^d} dk(\ell\cdot\nabla\omega(k))\omega(k)W_\tau(k,t) + \mathscr{O}(\lambda). \tag{36}$$

The next task is to take the limit $\tau\to 0$ in (31). One has $W_{\beta,0}(k) = (e^{\beta\omega(k)}-1)^{-1}$ which is a stationary solution of (34). Thus the limit $\tau\to 0$ amounts to linearize (35) at the equilibrium Wigner function

$$W_\beta(k) = (e^{\beta\omega(k)}-1)^{-1}, \tag{37}$$

to say

$$W_{\beta,\tau} = W_\beta + \tau W_\beta\tilde W_\beta(\ell\cdot\nabla\omega)\omega + \mathscr{O}(\tau^2). \tag{38}$$

Note that $\int dk(\nabla\omega)\omega W_\beta = 0$. As suggested by (38), with a significance which will become more convincing in the context of the Gaussian fluctuation theory, see Sect. 5, the natural linearization of $\mathscr{C}$ is

$$\mathscr{C}(W_\beta + \delta W_\beta\tilde W_\beta f) = -\delta Lf + \mathscr{O}(\delta^2). \tag{39}$$

From (35) one deduces

$$\begin{aligned}(Lf)_1 = \frac{\pi}{2}\int_{\mathbb{T}^{2d}} dk_2dk_3(\omega_1\omega_2\omega_3)^{-1}\\ \times(2\delta(\omega_1+\omega_2-\omega_3)\delta(k_1+k_2-k_3)\tilde W_{\beta1}\tilde W_{\beta2}W_{\beta3}(f_1+f_2-f_3)\\ +\delta(\omega_1-\omega_2-\omega_3)\delta(k_1-k_2-k_3)\tilde W_{\beta1}W_{\beta2}W_{\beta3}(f_1-f_2-f_3)).\end{aligned} \tag{40}$$

Properties of L will be discussed in the subsequent section.

Let A be the linear operator obtained from flat linearization as

$$\mathscr{C}(W_\beta + \delta f) = \delta A f + \mathscr{O}(\delta^2). \tag{41}$$

Clearly $A(W_\beta \tilde{W}_\beta f) = -Lf$. Combining (31) and (36) we finally conclude

$$\lim_{\lambda \to 0} \ell \cdot C_\lambda(\lambda^{-2} t)\ell = \ell \cdot C_{\mathrm{kin}}(t)\ell \tag{42}$$

with

$$\ell \cdot C_{\mathrm{kin}}(t)\ell = \langle (2\pi)^{-1}(\ell \cdot \nabla\omega)\omega,\ e^{-A|t|} W_\beta \tilde{W}_\beta (2\pi)^{-1}(\ell \cdot \nabla\omega)\omega \rangle, \tag{43}$$

where $\langle \cdot, \cdot \rangle$ is the inner product in $L^2(\mathbb{T}^d, dk)$.

For future use it will be convenient to write $C_{\mathrm{kin}}(t)$ in a more symmetric form. Expanding the exponential one notes that

$$\begin{aligned} \ell \cdot C_{\mathrm{kin}}(t)\ell = \big\langle & (2\pi)^{-1}(\ell \cdot \nabla\omega)\omega (W_\beta \tilde{W}_\beta)^{1/2}, \\ & \exp\big[-(W_\beta \tilde{W}_\beta)^{-(1/2)} L (W_\beta \tilde{W}_\beta)^{-(1/2)} |t|\big] \\ & \times (W_\beta \tilde{W}_\beta)^{1/2} (2\pi)^{-1}(\ell \cdot \nabla\omega)\omega \big\rangle. \end{aligned} \tag{44}$$

As will be shown, $L = L^*$, i.e. L is a symmetric operator in $L^2(\mathbb{T}^d, dk)$. Therefore $C_{\mathrm{kin}}(t)$ is a positive symmetric $d \times d$ matrix.

In the kinetic limit the thermal conductivity is given through

$$\begin{aligned} \ell \kappa_{\mathrm{kin}} \cdot \ell &= \beta^2 \int_0^\infty dt\, \ell \cdot C_{\mathrm{kin}}(t)\ell \\ &= (2\pi)^{-2} \beta^2 \langle (\ell \cdot \nabla\omega)\omega W_\beta \tilde{W}_\beta,\ L^{-1}(\ell \cdot \nabla\omega)\omega W_\beta \tilde{W}_\beta \rangle. \end{aligned} \tag{45}$$

Reversing our argument, and assuming uniformity in t for the limit $\lambda \to 0$, one infers that the true thermal conductivity, $\kappa(\lambda)$, of the anharmonic model behaves as

$$\kappa(\lambda) \cong \lambda^{-2} \kappa_{\mathrm{kin}} \tag{46}$$

for small λ.

In the classical limit $[a(k), a(k')^*] = 0$, i.e., $W = \tilde{W}$. In the definition of L one has thus to replace

$$W_\beta,\ \tilde{W}_\beta \quad \text{by} \quad W_\beta^{\mathrm{cl}}(k) = \frac{1}{\beta\omega(k)}. \tag{47}$$

We presented the argument for a cubic on-site potential. But, clearly, the result holds also for other small anharmonicities. Only the collision operator, and its linearization L, would have to be modified.

4 The Linearized Collision Operator

If one accepts the argument leading to (42), the remaining task is to study the spectral properties of the linearized collision operator, from which the time decay of $C_{\mathrm{kin}}(t)$ can be inferred. While this looks like a conventional mathematical physics problem, the difficulty comes from the energy-momentum constraint. Only in a few special cases there is an explicit solution. Otherwise one has to work with the implicit definition. In fact, there can be no solution at all, in which case $L = 0$, or several solutions, in which case one has to sum over all collision branches.

(i) *quadratic form*. For three phonon processes, on-site potential V_3, the quadratic form of the linearized collision operator $L = L_3$ is given by

$$\begin{aligned}\langle g, L_3 f\rangle = \frac{\pi}{2}\int_{\mathbb{T}^{3d}} dk_1 dk_2 dk_3 (\omega_1\omega_2\omega_3)^{-1}\delta(\omega_1+\omega_2-\omega_3)\delta(k_1+k_2-k_3)\\ \times W_{\beta 1}W_{\beta 2}\tilde{W}_{\beta 3}(g_1+g_2-g_3)(f_1+f_2-f_3).\end{aligned} \tag{48}$$

Correspondingly for the on-site potential V_4 one has

$$\begin{aligned}\langle g, L_4 f\rangle &= \frac{3\pi}{4}\cdot\frac{3}{4}\int dk_1 dk_2 dk_3 dk_4 (\omega_1\omega_2\omega_3\omega_4)^{-1}\\ &\quad\times \delta(\omega_1+\omega_2-\omega_3-\omega_4)\delta(k_1+k_2-k_3-k_4)\\ &\quad\times W_{\beta 1}W_{\beta 2}\tilde{W}_{\beta 3}\tilde{W}_{\beta 4}(g_1+g_2-g_3-g_4)(f_1+f_2-f_3-f_4)\\ &\quad+\frac{3\pi}{4}\int dk_1 dk_2 dk_3 dk_4 (\omega_1\omega_2\omega_3\omega_4)^{-1}\delta(\omega_1+\omega_2+\omega_3-\omega_4)\\ &\quad\times \delta(k_1+k_2+k_3-k_4)W_{\beta 1}W_{\beta 2}W_{\beta 3}\tilde{W}_{\beta 4}(g_1+g_2+g_3-g_4)\\ &\quad\times (f_1+f_2+f_3-f_4)\\ &= \langle f, L_{4\mathrm{p}} f\rangle + \langle f, L_{4\mathrm{t}} f\rangle.\end{aligned} \tag{49}$$

$L_{4\mathrm{p}}$ corresponds to the collision of a pair of phonons and $L_{4\mathrm{t}}$ to a merger of three phonons into a single one, and its time reversal. The quadratic forms for L_3, $L_{4\mathrm{p}}$, $L_{4\mathrm{t}}$ (for notational simplicity from now on commonly denoted by L) are somewhat formal. Firstly, if $\omega(0) = 0$ and $\omega(k) > 0$ otherwise, the smooth functions g, f have to vanish at $k = 0$. More seriously, the proper definition of the δ-function requires to study more carefully the solutions to the energy constraint

$$\omega(k_1) + \omega(k_2) = \omega(k_1 + k_2), \tag{50}$$

say in the case of L_3. For the purpose of our exposition, let us simply assume that the quadratic form defines L as a self-adjoint operator. Clearly, $L \geq 0$ since $\langle f, Lf\rangle \geq 0$. As $(\ell\cdot\nabla\omega)\omega$ is bounded, one has

$$\ell\cdot C_{\mathrm{kin}}(t)\ell \leq (2\pi)^{-2}\langle(\ell\cdot\nabla\omega)\omega, (\ell\cdot\nabla\omega)\omega\rangle. \tag{51}$$

(ii) *zero subspace*. To establish that $\lim_{t\to\infty} C_{\mathrm{kin}}(t) = 0$, $(\ell\cdot\nabla\omega)\omega$ has to be orthogonal to the zero subspace of L. There seems to be no cheap argument and one has to study the solutions to

$$Lf = 0. \tag{52}$$

From (48), (49) it follows that f has to be a collisional invariant, see [13, 14] for the definition. Considering only the first summand of (49), there is a general argument [14], that the solutions to $\langle f, L_{4\mathrm{p}} f\rangle = 0$ are spanned by 1, ω. Note that $\langle 1, (\ell\cdot\nabla\omega)\omega\rangle = 0$, $\langle \omega, (\ell\cdot\nabla\omega)\omega\rangle = 0$. The constant function results from phonon number conservation in a pair collision. This conservation law will be destroyed by adding a little bit of either three-phonon, L_3, or the second term of the four-phonon processes, $L_{4\mathrm{t}}$. The zero subspace is then one-dimensional and spanned by ω only. For L_3 of (48), the classification of the collisional invariants is an open problem.

(iii) *spectral gap*. If L has a spectral gap, the energy current correlation decays exponentially. If in addition $(\ell\cdot\nabla\omega)\omega$ is orthogonal to the zero subspace of L, then the conductivity, as the time-integral over $C_{\mathrm{kin}}(t)$, is finite (and non-zero). In particular (46) holds.

L is a sum of a multiplication operator and an integral operator,

$$L = V + I, \qquad Vf(k) = V(k)f(k), \qquad If(k) = \int_{\mathbb{T}^d} dk' I(k,k') f(k'), \tag{53}$$

where, say in the case of L_3,

$$\begin{aligned} V(k) = \frac{\pi}{2} W_\beta(k)\omega(k)^{-1} \int_{\mathbb{T}^d} dk_1 \big(\omega(k_1)\omega(k+k_1)\big)^{-1} \\ \times \big(2\delta(\omega(k)+\omega(k_1)-\omega(k+k_1)) W_\beta(k_1)\tilde{W}_\beta(k+k_1) \\ + \delta(\omega(k)-\omega(k_1)-\omega(k+k_1))\tilde{W}_\beta(k_1)\tilde{W}_\beta(k+k_1)\big). \end{aligned} \tag{54}$$

The integral kernel $I(k,k')$ is implicitly defined. It has no definite sign and tends to be divergent on lower-dimensional submanifolds of $\mathbb{T}^d\times\mathbb{T}^d$. It would be useful to know under what conditions the integral operator I is compact.

In the very common relaxation time approximation, I is simply dropped and one sets in approximation

$$\ell\cdot C_{\mathrm{kin}}(t)\ell = (2\pi)^{-2}\langle (\ell\cdot\nabla\omega)\omega, e^{-|t|/\tau} W_\beta \tilde{W}_\beta (\ell\cdot\nabla\omega)\omega\rangle \tag{55}$$

with the relaxation time

$$\tau(k) = W_\beta(k)\tilde{W}_\beta(k) V(k)^{-1}, \tag{56}$$

see (44).

(iv) *FPU chains*. The Fermi-Pasta-Ulam chain is the special case $d = 1$ with nearest neighbor coupling and no quantization. For a harmonic on-site potential the dispersion relation is $\omega(k) = (\omega_0^2 + 1 - \cos(2\pi k))^{1/2}$, $k\in\mathbb{T}$. Although $d = 1$, the conservation laws of energy and momentum allow for non-degenerate pair collision

and $L_{4p} \neq 0$, while $L_{4t} = 0$ [10, 1, 4]. There are fairly explicit formuli for the potential V and the integral kernel I [3]. For $\omega_0 > 0$ and a quartic on-site potential V_4, the linearized collision operator has a gap and the zero subspace is two-dimensional. The gap seems to close as $\omega_0 \to 0$. On the basis of numerical simulations, the conductivity should be finite even for $\omega_0 = 0$ [1]. The FPU-β chain has the nonlinearity V_{di4}. V and I has been computed by Pereverzev [10]. He uses the relaxation time approximation and finds that $C_{kin}(t) \cong t^{-3/5}$ for large t. Using a resolvent expansion, in [4] we prove corresponding sharp bounds and thereby confirm the relaxation time approximation in this particular case. For a finite chain of length N with thermal reservoirs at both ends, the energy transport is then anomalous and the thermal conductivity diverges as $N^{2/5}$, which seems to be in agreement with molecular dynamics. For a more detailed discussion we refer to [2], Sect. 6.

5 Gaussian Fluctuation Theory

Energy transport can be viewed in the more general context of time-dependent Gaussian fluctuation theory close to thermal equilibrium. For low density gases this link is reviewed in [11] with further examples discussed in [12]. The purpose of this section is to explain how phonon kinetic theory makes no exception. In [11, 12] spatial variation is included. Since our exposition deals only with the spatially homogeneous system, we stick to such a set-up also for the fluctuation theory.

Physically, one considers time-dependent fluctuations in equilibrium for the number of phonons with wave number k. Technically one has to sum over phonons in a small volume element in k-space. To be more precise we partition the tours $\mathbb{T} = [-1/2, 1/2]$ by a grid with spacing ε and denote it by $\mathbb{T}_\varepsilon$. $(\mathbb{T}_\varepsilon)^d$ corresponds to the crystal volume $[1, \dots, l]^d \subset \mathbb{Z}^d$ with periodic boundary conditions, $l = 1/\varepsilon$. Let $f : \mathbb{T}^d \to \mathbb{R}$ be a smooth test function. Then the fluctuation field, indexed by f and t, is defined through

$$\xi^\varepsilon(f,t) = \varepsilon^{d/2} \sum_{k \in (\mathbb{T}_\varepsilon)^d} f(k)\big(a^\varepsilon(k,t)^* a^\varepsilon(k,t) - \langle a^\varepsilon(k)^* a^\varepsilon(k)\rangle_\beta\big). \tag{57}$$

$a^\varepsilon(k,t)$ depends on ε through the finite crystal volume ε^{-d}, through setting $\lambda^2 = \varepsilon$, and through the rescaled time $\varepsilon^{-1}t$ in microscopic units. The claim is that, in distribution, the limit

$$\lim_{\varepsilon \to 0} \xi^\varepsilon(f,t) = \xi_t(f) \tag{58}$$

exists and that the limit random field $\xi_t(f)$ is classical. In fact, the limit field should be jointly Gaussian and governed by the linear Langevin equation

$$\frac{\partial}{\partial t}\xi_t(k) = A\xi_t(k) + B\eta_t(k), \tag{59}$$

where $\xi_t(f) = \int_{\mathbb{T}^d} dk f(k)\xi_t(k)$. A is the generator from the linearized Boltzmann equation, compare with (41), and η_t is normalized Gaussian white noise with

$$\mathbb{E}(\eta_t(k)\eta_{t'}(k')) = \delta(t-t')\delta(k-k'). \tag{60}$$

The linear operator B controls the strength and correlations for the noise input to the various k-modes.

The main observation of the fluctuation theory is the relationship between A and B through the equal-time equilibrium fluctuations. We set, as a linear operator,

$$\langle g,\ Cf\rangle = \lim_{\varepsilon\to 0}\langle \xi^\varepsilon(g,0)\xi^\varepsilon(f,0)\rangle_\beta. \tag{61}$$

Using that

$$\begin{aligned}&\langle a^*(k_1)a(k_2)a^*(k_3)a(k_4)\rangle_\beta - \langle a^*(k_1)a(k_2)\rangle_\beta\langle a(k_3)^*a(k_4)\rangle_\beta\\ &\delta(k_1-k_4)\delta(k_2-k_3)W_\beta(k_1)\tilde W_\beta(k_2),\end{aligned} \tag{62}$$

one obtains

$$\langle g,\ Cf\rangle = \int_{\mathbb{T}^d} dk g(k)W_\beta(k)\tilde W_\beta(k)f(k), \tag{63}$$

in other words C is the operator of multiplication by $W_\beta\tilde W_\beta$. The fluctuation-dissipation relation takes then the form

$$AC + CA^* = -BB^*. \tag{64}$$

Since $AC = L = L^* = CA^*$, one concludes that the noise strength is

$$BB^* = 2L. \tag{65}$$

A posteriori this identity explains also the at first sight unexpected linearization in (39). Only then the linearized operator is symmetric, as is obvious from (65).

Solving (59), the covariance of the stationary fluctuation field is given by

$$\langle \xi_t(g)\xi_0(f)\rangle = \langle g,\ e^{A|t|}Cf\rangle, \tag{66}$$

in agreement with the special case $f = g = (2\pi)^{-1}(\ell\cdot\nabla\omega)\omega$ of interest in Sect. 4.

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Metastates, Translation Ergodicity, and Simplicity of Thermodynamic States in Disordered Systems: an Illustration

Charles M.Newman and Daniel L. Stein

Abstract In the context of short-range Edwards-Anderson spin glasses, we propose an approach to obtaining rigorous results based on combining the use of metastates, translation-ergodicity and the dependence of certain quantities on small changes of one or more couplings (or fields). This seems especially suited to showing that the structure of thermodynamic states cannot be too complex. As an illustration, we use this approach to prove that thermodynamic states appearing in (e.g.) the periodic boundary condition metastate cannot decompose into a number of pure state pairs strictly between one and infinity.

1 Introduction

The statistical mechanics, equilibrium and nonequilibrium, of systems with quenched disorder, of which spin glasses are a prototype, present a rich array of open problems. As demonstrated in previous work of the authors [14–32], some of the central questions for short-range systems are amenable to rigorous analysis. However, it remains uncertain whether spin glasses possess nontrivial equilibrium properties and their study presents numerous mathematical challenges, some of which we address here.

Most theoretical investigations take as a starting point the Edwards-Anderson (EA) Ising Hamiltonian [6]:

Charles M.Newman
Courant Institute of Mathematical Sciences, New York University, New York, NY 10012, USA, e-mail: newman@courant.nyu.edu

Daniel L. Stein
Physics Department and Courant Institute of Mathematical Sciences, New York University, New York, NY 10012, USA, e-mail: daniel.stein@nyu.edu

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$$\mathscr{H} = -\sum_{<x,y>} J_{xy}\sigma_x\sigma_y - h\sum_x \sigma_x, \tag{1}$$

where x is a site in Z^d, $\sigma_x = \pm 1$ is the spin at site x, the spin couplings J_{xy} are independent, identically distributed random variables, h is an external magnetic field, and the first sum is over nearest neighbor pairs of sites only. We will choose $h = 0$ and the J_{xy} to be taken from the standard normal distribution $\mathscr{N}(0, 1)$; consequently, (1) has global spin inversion symmetry.

A pure phase α of an EA spin glass (at a sufficiently low temperature T in a sufficiently high dimension d) should then be characterized by a vanishing magnetization per spin

$$\langle M\rangle_\alpha = \lim_{L\to\infty} \frac{1}{|\Lambda_L|}\sum_{x\in\Lambda_L} \langle\sigma_x\rangle_\alpha \tag{2}$$

accompanied by a nonvanishing "EA order parameter,"

$$q_{EA} = \lim_{L\to\infty} \frac{1}{|\Lambda_L|}\sum_{x\in\Lambda_L} \langle\sigma_x\rangle_\alpha^2, \tag{3}$$

where Λ_L is a cube of side length L and volume $|\Lambda_L|$ centered at the origin, and $\langle\cdot\rangle_\alpha$ denotes a thermal average in the pure state α. It is generally assumed that q_{EA}, which depends on d and T, is independent of α.

2 The Sherrington-Kirkpatrick Model and the Parisi Replica Symmetry Breaking Solution

The Sherrington-Kirkpatrick (SK) model [35] is an infinite-range version of the EA model in which mean field theory is presumably exact. For a system of N spins in zero field the SK Hamiltonian is

$$\mathscr{H}_N = -(1/\sqrt{N})\sum_{1\le i<j\le N} J_{ij}\sigma_i\sigma_j, \tag{4}$$

where the couplings J_{ij} are again i.i.d. $\mathscr{N}(0, 1)$ r.v.'s. This model has a sharp phase transition at $T_c = 1$ [35] (see also [7, 39]).

The low-temperature phase has an unusual thermodynamic structure, worked out by Parisi and collaborators in a series of papers [33, 34, 10, 11]. Following the procedures underlying the analysis, it came to be known as *replica symmetry breaking* (RSB). The main features of this structure include an infinity of pure thermodynamic states [34] with the features of non-self-averaging and ultrametricity of spin overlap functions [10, 11]. For details see [3, 4, 12, 36, 5]. A number of features (though not all) of the Parisi solution for the SK model have been rigorously verified; see, for example [2, 7, 37–39]. Many workers in the field now believe that

the essential physical features of the low-temperature phase of the SK model are understood.

3 Open Problems

For the more realistic EA model, the nature of the low-temperature phase, or even the existence of such a phase, remains open, even from a nonrigorous physics standpoint. Some of the basic open questions are:

Does the EA Ising model really have an equilibrium phase transition above some lower critical dimension d_c?

If the answer to the above question is yes, is the spin-flip symmetry broken in the low-temperature phase (i.e., is $q_{EA} > 0$)?

If the answer to both of the above questions is yes, what is the number of equilibrium pure state pairs for $0 < T < T_c(d)$ and ground state pairs (at $T = 0$)?

If there exist infinitely many equilibrium pure states in some dimensions and at some temperatures, are they organized according to the mean-field RSB picture (i.e., nontrivial mixtures of pure states with non-self-averaging and ultrametricity of overlaps)?

We have argued [18, 19, 28, 29] that the proper mathematical tool to address these last two questions (which we hereafter focus on) is the *metastate.*

4 Metastates

Consider an EA spin glass with fixed coupling realization, hereafter denoted $\mathscr{J}$. If there exist many pure states, a sequence of volumes Λ_L with boundary conditions chosen independently of the couplings will generally *not* converge to a limiting thermodynamic state, in the sense that correlations $\langle \sigma_{i_1} \cdots \sigma_{i_n} \rangle^L$, computed in Λ_L from the finite-volume Gibbs state (with, e.g., periodic boundary conditions), will not have a single limit as $L \to \infty$ but rather many different limits along different subsequences of L's (necessarily chosen in a $\mathscr{J}$-dependent manner). We have called this phenomenon *chaotic size dependence* [14]. Such behavior in L is analogous to chaotic behavior in time t along the orbit of a dynamical system: the behavior of any particular orbit is deterministic but effectively unpredictable, appearing to be a random sample from some distribution κ on the state space of the dynamical system. Nevertheless, one can in principle reconstruct κ by keeping a record of the proportion of time the particle spends in each coarse-grained region of state space. Similarly, one can prove [18, 19] that for inhomogeneous (disordered) systems like spin glasses, a similar distribution exists: roughly speaking, the fraction of Λ_L's in which a given thermodynamic state Γ appears converges. The state Γ can be either pure or mixed, depending on the boundary conditions.

Mathematically, a metastate κ is a probability measure on the space of all (fixed $\mathscr{J}$) thermodynamic states. Of course, the metastate depends on the boundary conditions used: we will refer to the metastate constructed from a deterministic sequence of volumes, all with periodic boundary conditions, as the "periodic b.c. metastate", and similarly for the antiperiodic b.c. metastate, the free b.c. metastate, and so on. One can also construct metastates in which the b.c.'s vary with L.

A simplified empirical construction of κ would be as follows: consider a "microcanonical" ensemble κ_L, in which each of the finite volume Gibbs states $\rho^{(1)}, \ldots, \rho^{(L)}$ in volumes $\Lambda_1, \ldots, \Lambda_L$ has weight L^{-1}. Then $\kappa = \lim_{L\to\infty} \kappa_L$. The meaning of the limit is that for every well-behaved function $g(\cdot)$ on states,

$$\lim_{L\to\infty} L^{-1} \sum_{\ell=1}^{L} g(\rho^{(\ell)}) = \{g(\Gamma)\}_\kappa, \tag{5}$$

where the bracket $\{.\}_\kappa$ denotes the average over the metastate κ.

There is an alternative (and earlier) construction due to Aizenman and Wehr [1], where one replaces the microcanonical ensemble κ_L by the ensemble of states obtained by varying the couplings *outside* Λ_L. Here, for every well-behaved function F of finitely many couplings and finitely many correlations,

$$\lim_{L\to\infty} [F(\mathscr{J}, \rho^{(L)})]_{av} = \left[\{F(\mathscr{J}, \Gamma)\}_{\kappa(\mathscr{J})}\right]_{av}, \tag{6}$$

where $[.]_{av}$ denotes the average over the quenched coupling distribution. It has not been proved that these relatively simple limits, using all ℓ's and L's, exist, but it can be proved [19] that there exist deterministic (i.e., $\mathscr{J}$-independent) subsequences of ℓ's and L's for which limits such as in both (5) and (6) exist and yield the *same* $\kappa(\mathscr{J})$. (In some cases these subsequences may need to be sparse; see, e.g., [8, 9].)

5 Invariance and Ergodicity

The metastate is a central tool we will use to analyze whether the type of ordering present in the RSB solution of the SK model can hold in more realistic short-ranged models. We will combine it with some basic invariance and ergodicity properties of functions on the disorder random variables to draw rigorous conclusions about some of these functions that are of physical and mathematical interest.

Our results basically apply to any disorder distribution $\nu(\mathscr{J})$ in which the couplings are independent, identically distributed random variables (although parts of the arguments are most easily carried out when each coupling has a continuous distribution as in the Gaussian case). At some fixed dimension d and temperature T, consider a function $\mathscr{F}(d, T, \mathscr{J})$ on Z^d that is translation-invariant on the couplings in at least one coordinate. For example, $\mathscr{F}(d, T, \mathscr{J})$ might denote the number of pure states, or the spin overlap function [12] or the sum of the squares of the pure state weights (if there are a countable number of pure states) averaged over the

metastate. Then it can be proved that $\mathscr{F}(d, T, \mathscr{J})$ is constant in $\mathscr{J}$ almost surely; i.e., it is the same for a.e. $\mathscr{J}$, at fixed T and d. Of course, $\mathscr{F}(d, T, \mathscr{J})$ can have some dependence on both d and T. It also can depend on ν, although that dependence is not explicitly indicated. But once all of these are determined, it cannot depend on any realization $\mathscr{J}$ of the couplings (outside of a set of measure zero). In the language of spin glass theory, $\mathscr{F}$ is a self-averaged quantity.

The proof of such a statement lies in a straightforward use of the ergodic theorem [13], and depends on three ingredients: measurability of $\mathscr{F}$ as a function of $\mathscr{J}$, translation-invariance of $\mathscr{F}$ with respect to a uniform shift of the xy indices of the couplings, and translation-ergodicity of the underlying disorder distribution ν. By the ergodic theorem, any (measurable) translation-invariant function of $\mathscr{J}$ chosen from a translation-ergodic distribution is constant almost surely (that is, is the same for a.e. realization of $\mathscr{J}$). Now the couplings J_{xy} are independent, identically distributed random variables. The distribution for such random variables is translation-ergodic [40], and so $\nu(\mathscr{J})$ is translation-ergodic. So, because $\mathscr{F}$ is a translation-invariant function of $\mathscr{J}$, which is drawn from the translation-ergodic distribution $\nu(\mathscr{J})$, it follows that $\mathscr{F}$ is the same for a.e. $\mathscr{J}$ (at fixed T and d). We note that although this line of reasoning might be regarded as trivial from a probability or ergodic theory perspective, it seems to lead to physically nontrivial consequences.

This reasoning can be used to rule out the "standard" RSB picture [16, 29], in which an infinite-volume thermodynamic mixed state is constructed, its overlaps taken, and the resulting distribution on the overlaps shown to be self-averaging. However, the metastate allows one to construct alternative scenarios, and one of these—the "nonstandard" RSB picture, although different from the usual version of the mean-field scenario, represents the maximal allowable low-temperature structure that still retains some features of the Parisi solution. Its properties are described in [18, 19, 29]. A further property of the metastate, that of invariance with respect to gauge-related boundary conditions [21], renders the nonstandard RSB picture highly implausible. But a complete proof ruling it out remains to be found. In the next section we add one more ingredient—manipulation of couplings (and/or fields) that we hope might lead to further progress both in resolving not only this question, but also others, such as numbers of pure states.

6 A Strategy for Rigorous Studies of Spin Glasses

The previous discussion points towards a strategy for obtaining rigorous results on spin glasses and other systems with quenched disorder. Given a suitable Hamiltonian, such as (1), the first step is to construct an appropriate metastate. Because translation-invariance and ergodicity are crucial ingredients, it is often easiest to use a manifestly translation-covariant construction, such as the periodic boundary condition metastate. (However, with a little more work, many other boundary conditions, such as free or fixed, can be used [26].) The next step is to choose some

translation-invariant function $\mathscr{F}$ on the couplings (and/or fields, if present), as described in Sect. 5. The final step is to manipulate finitely many couplings (or fields) by a finite amount (so that the resulting set of realizations remains of nonzero measure) in such a way as to change $\mathscr{F}$ (unless the metastate has a simple enough structure), leading to a contradiction. Such a strategy (or more accurately, a variant of it), was employed in studying ground state incongruence in $2D$ EA models [25, 26].

As an illustration, we will show how this procedure can be used to prove a moderately interesting result (valid in any finite dimension) restricting the nature of a putative low-temperature spin glass phase. Consider the periodic boundary condition metastate of the Hamiltonian (1) in zero field, and suppose further that this metastate is supported on many thermodynamic states Γ, with each Γ comprising a countable decomposition into pure states:

$$\Gamma(\sigma) = \sum_{\alpha} W_\alpha \rho_\alpha(\sigma), \tag{7}$$

where $W_\alpha = W_\alpha(\Gamma)$ is the weight of pure state $\rho_\alpha(\sigma)$ in Γ. We will show how to prove that for every Γ (more precisely, for a.e. Γ in the metastate), the above decomposition consists of either a single pair or infinitely many. The theorem does not rule out the possibility that some Γ's in the metastate comprise a single pure state pair while others consist of infinitely many.

We note that a similar but somewhat different result was proved in [31] using other methods—namely, that if the periodic b.c. metastate is supported on Γ's with some having nontrivial decompositions into multiple pure state pairs, then the *entire* metastate is supported on an *uncountable* infinity of pure states. This latter result does not address the distribution of pure states within the different Γ's that together constitute the support of the metastate.

We will make an assumption that is not needed but which simplifies and shortens the proof; namely, that if E_{L_0} is the edge set in Λ_{L_0}, then the spatially averaged quantity $e_{EA} = \lim_{L_0\to\infty} |E_{L_0}|^{-1} \sum_{\langle xy\rangle\in E_{L_0}} \langle\sigma_x\sigma_y\rangle_\alpha^2$ is independent of α. (Note that this is just a two-spin generalization of the analogous one-spin formula (3), where the assumption of independence with respect to α is standard.)

We now sketch the proof of the claim made above. Suppose that a nonzero fraction of Γ's in the metastate (i.e., a set of Γ's with strictly positive metastate measure) are decomposable according to (7) into a finite number (greater than one) of pure state pairs. Consider a function $\mathscr{F}(\Gamma)$ on the states Γ (or equivalently, on the correlation functions that characterize Γ). The average of $\mathscr{F}$ over the entire metastate is

$$\overline{\mathscr{F}}(\mathscr{J}) = \int d\kappa_{\mathscr{J}}(\Gamma)\mathscr{F}(\Gamma). \tag{8}$$

If $\overline{\mathscr{F}}(\mathscr{J})$ is a (measurable) translation-invariant function of the coupling realization $\mathscr{J}$, then by the (spatial) ergodic theorem it must be the same for almost every $\mathscr{J}$, as discussed above.

One $\mathscr{F}(\Gamma)$ leading to such an $\overline{\mathscr{F}}$ is the quantity (for ease of notation, dependence on $\mathscr{J}$ is hereafter dropped)

$$\mathscr{F}^{(n)}(\Gamma) = \frac{1}{n}\sum_{\alpha} W_\alpha^n, \tag{9}$$

where $n > 0$ need not be an integer and the index α will refer to a globally flip-related pure state pair with W_α denoting the sum of the weights of the two states in the pair. Thus $0 \le W_\alpha \le 1$ for every α in Γ and $\sum_\alpha W_\alpha = 1$ for every Γ.

We will now suppose that every Γ consists of only *finitely* many pure state pairs with an upper bound on the number of pairs as Γ varies over the metastate and with a nonzero fraction having more than a single pair. These assumptions can be substantially weakened, as we explain later, by a slight modification of the arguments. For some fixed $\mathscr{J}$, we choose an arbitrary bond $\langle xy\rangle$ and change its coupling value by a finite amount: $J_{xy} \to J'_{xy} = J_{xy} + \Delta J_{xy}$. In any Γ, every pure state pair α transforms [1] (see also [19–21, 28, 29]) to a new pure state pair (also denoted α), with corresponding weight transformation

$$W_\alpha \to W'_\alpha = r_\alpha W_\alpha / \sum_\gamma r_\gamma W_\gamma \tag{10}$$

where

$$r_\alpha = \Big\langle \exp(\beta \Delta J_{xy}\sigma_x\sigma_y)\Big\rangle_\alpha. \tag{11}$$

For notational simplicity we will absorb the inverse temperature β into ΔJ_{xy} from here on. Now consider the derivative of $\mathscr{F}^{(n)}(\Gamma)$ with respect to ΔJ_{xy}, evaluated at $\Delta J_{xy} = 0$. A straightforward calculation gives

$$\frac{\partial \mathscr{F}^{(n)}(\Gamma)}{\partial(\Delta J_{xy})}\Big|_{\Delta J_{xy}=0} = \sum_\alpha W_\alpha^n \Big(\langle\sigma_x\sigma_y\rangle_\alpha - \langle\sigma_x\sigma_y\rangle_\Gamma\Big), \tag{12}$$

where $\langle\sigma_x\sigma_y\rangle_\Gamma = \sum_\alpha W_\alpha \langle\sigma_x\sigma_y\rangle_\alpha$. The second derivative is

$$\begin{aligned}\frac{\partial^2 \mathscr{F}^{(n)}(\Gamma)}{\partial(\Delta J_{xy})^2}\Big|_{\Delta J_{xy}=0} = \sum_\alpha W_\alpha^n \Big[& n\Big(\langle\sigma_x\sigma_y\rangle_\alpha - \langle\sigma_x\sigma_y\rangle_\Gamma\Big)^2 \\ & + \langle\sigma_x\sigma_y\rangle_\Gamma^2 - \langle\sigma_x\sigma_y\rangle_\alpha^2\Big].\end{aligned} \tag{13}$$

The 'average' edge overlap in Γ is

$$\begin{aligned} e_\Gamma &= \lim_{L_0\to\infty} |E_{L_0}|^{-1} \sum_{\langle xy\rangle\in E_{L_0}} \langle\sigma_x\sigma_y\rangle_\Gamma^2 \\ &= \lim_{L_0\to\infty} |E_{L_0}|^{-1} \sum_{\langle xy\rangle\in E_{L_0}} \sum_{\alpha\beta} W_\alpha W_\beta \langle\sigma_x\sigma_y\rangle_\alpha \langle\sigma_x\sigma_y\rangle_\beta. \end{aligned} \tag{14}$$

By assumption, e_{EA} (defined earlier) is independent of α; it is also nonzero since $T < \infty$. Then by a Cauchy-Schwarz inequality, $e_\Gamma \le e_{EA}$ with the equality holding if and only if Γ consists of a single pure state pair.

We now use the assumption that a nonzero fraction of Γ's have a nontrivial pure state pair decomposition, and therefore have $e_\Gamma < e_{EA}$. It is then easy to see that the spatially averaged second derivative of $\overline{\mathscr{F}^{(n)}}$ approaches a strictly negative limit as $n \to 0$. This means that it must have taken a negative value *before* the limit was reached—i.e., for some small $n > 0$. We have therefore shown that for sufficiently small $n > 0$ the value of the spatially averaged second derivative of the integrand in (8) with $\mathscr{F}(\Gamma)$ given by (9) is strictly negative if a nonzero fraction of Γ's have finitely many (but more than one) pure state pairs. This in turn implies that there would be a nontrivial dependence on $\mathscr{J}$ of a translation-invariant quantity, leading to a contradiction with ergodicity.

One might wonder why the above result can't be extended to rule out Γ's whose decompositions have an infinite number of pure states. However, when $n \to 0$, the second derivative of $\mathscr{F}^{(n)}(\Gamma)$ given by (13) is guaranteed to remain finite for every Γ only if all Γ's have a decomposition into a finite number of pure state pairs. By extension, the site-averaged second derivative of $\overline{\mathscr{F}^{(n)}}$ is guaranteed to remain finite, and more significantly to be negative for some small $n > 0$. One might then ask about ruling out situations where Γ's can have an infinite set of pure states by considering a quantity such as $\mathscr{F}^{(n)}(\Gamma)$, but with the sum in (9) restricted to a finite number of pure state pairs (e.g., the ten pairs in each Γ with largest weight), and then using similar arguments as above. The problem with that approach, which we have not yet overcome, is that as one varies the individual couplings, the "identity" of the ten maximal weight states can change discontinuously so (10)–(11) do not apply. This leads to the need to analyze the "internal boundaries" in the support of the metastate where there is more than one pure state tied for the tenth largest weight and to understand the nature of their contribution to some modified version of (13).

As stated, our proof doesn't rule out the possibility that one could have a situation where Γ's with a decomposition into a finite number of pure state pairs might coexist with Γ's with a decomposition into an *infinite* number of pure state pairs (because then $\overline{\mathscr{F}^{(n)}}$ isn't guaranteed to be finite). However, this is easily handled by redefining $\mathscr{F}^{(n)}(\Gamma)$ to equal 0 for Γ's with an infinite set of pure states; otherwise, it remains as defined in (9). The argument then goes through as before. Similarly, this type of modification allows one to remove the assumption that the number of pure state pairs in Γ is bounded as Γ varies over the metastate.

The only remaining issue is the assumption that an extended "bond" version of the EA order parameter was assumed to be independent of α. With more work, this assumption can be dropped, but we do not present the argument here.

7 Summary

In this note, we first reviewed some of the open questions concerning the structure of thermodynamic states at low temperature in disordered finite-dimensional systems such as the Edwards-Anderson spin glass. We then discussed the use of metastates and translation-ergodicity with respect to changes of the basic disorder variables, such as the couplings or fields. To illustrate the potential use of this approach to rigorously prove that the thermodynamic state structure cannot be too complicated (in arbitrary dimensions and temperatures), we showed how to prove by these methods that the thermodynamic states appearing in the metastate cannot have nontrivial decompositions into finitely many pure states.

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Random Matrices, Non-intersecting Random Walks, and Some Aspects of Universality

Toufic M. Suidan

Abstract The connection between various probabilistic and combinatorial models on the one hand and random matrices on the other hand is often understood through non-intersecting random walk descriptions of the quantities of interest. Two prominent distributions which appear in the fluctuation theory of both random matrices and models such as last passage percolation, longest increasing subsequence of random permutations, random tilings of the ABC-hexagon, and various non-intersecting walk ensembles are the GUE Tracy-Widom and sine kernel distributions. In this paper, we describe several of these models and related questions pertaining to the universality of these distributions.

1 Introduction

The last decade has seen an abundance of research activity at the interface of random matrix theory (RMT), combinatorics, number theory, probability, stochastic processes, statistics, and applied mathematics (see, for example [7, 37, 55, 20, 41] and the references within). In this paper we select a number of probabilistic and combinatorial models, connected to random matrices, whose analysis can be approached by first associating a non-intersecting random walk ensemble to the model and then analyzing this ensemble as the number of walkers grows. In particular, we will discuss the longest increasing subsequence of a random permutation, last passage percolation, random tiling of the ABC-hexagon, and collections of non-intersecting Brownian motions.

These models are exactly solvable in certain regimes. However, several of the models can be formulated in greater generality leading to questions of universality analogous to those of the central limit theorem of classical probability theory. Al-

Toufic M. Suidan
Department of Mathematics, The University of Arizona, 617 N. Santa Rita Ave., P.O. Box 210089, Tucson, AZ 85721-0089, USA, e-mail: tsuidan@math.arizona.edu

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though there are many seminal results in the context of Orthogonal and Symplectic ensembles (see for example [54, 3, 4, 2, 24]), we will focus exclusively on models in the "universality class" of the Gaussian Unitary ensemble.

1.1 Selected Basic Facts from Random Matrix Theory

The most prominent ensemble of $N \times N$ random matrices is the Gaussian Unitary Ensembe, GUE(N), which consists of the $N \times N$ Hermitian matrices equipped with the probability measure $\mathbb{P}^{(N)}(dH) = \frac{1}{\mathscr{Z}_N} e^{-Tr(H^2)} dH$ where $\mathscr{Z}_N$ is a normalizing constant. Denote the eigenvalues of H by $\lambda_1(H) \geq \cdots \geq \lambda_N(H)$. Define the kernels

$$\mathbb{A}(x, y) = \frac{Ai(x)Ai'(y) - Ai'(x)Ai(y)}{x - y} \qquad \mathbb{S}(x, y) = \frac{\sin(\pi(x - y))}{\pi(x - y)}, \quad (1)$$

where $Ai(x)$ is the classical Airy function. Two probability distribution functions of particular significance are expressed in terms of the following Fredholm determinants:

$$F_{TW}(\xi) = \det(1 - \mathbb{A})_{L^2(\xi,\infty)} \qquad F_{Sine}(\eta) = \det(1 - \mathbb{S})_{L^2[-\eta,\eta]}. \quad (2)$$

The Tracy-Widom distribution, F_{TW}, is the limiting distribution of the correctly scaled largest eigenvalue of a GUE random matrix as the size of the matrix grows [53, 55]:

$$\lim_{N\to\infty} \mathbb{P}^{(N)}\left(N^{\frac{1}{6}}(\lambda_1(H) - \sqrt{2N}) \leq x\right) = F_{TW}(x). \quad (3)$$

F_{Sine} is the limiting distribution for the gap probability of the eigenvalues 'in the bulk' of the spectrum:

$$\lim_{N\to\infty} \mathbb{P}^{(N)}\left(\lambda_i(H) \notin \left[\frac{-x}{\sqrt{2N}}, \frac{x}{\sqrt{2N}}\right] \text{ for all } i\right) = F_{Sine}(x). \quad (4)$$

1.2 The Karlin-McGregor Formula

The Karlin-McGregor formula [36] and related arguments are useful when calculating probabilities connected to non-intersecting Markov processes. Loosely speaking, this formula applies to one dimensional Markov processes whose ordering cannot change unless two paths have a moment of incidence. For example, the Karlin-McGregor formula applies to non-intersecting one dimensional diffusions. It also applies to non-intersecting simple symmetric random walks whose initial positions are on the lattice $2\mathbb{Z}$. However, it does not apply to simple symmetric random walks whose initial positions are at general locations on $\mathbb{Z}$ as this ensemble of walkers

can exchange ordering without having to be incident at some moment of time prior to the exchange. In this paper, we discuss a variety of situations in which Karlin-McGregor type arguments play a prominent role.

We state the Karlin-McGregor formula without proof. However, we stress that the arguments used to prove this formula apply to more general situations than those of the theorem and are often referred to as Lindström-Gessel-Viennot type arguments [28, 39, 51].

Theorem 1 (Karlin-McGregor). *Let $X_t^{(1)}, \dots, X_t^{(N)}$ be independent identically distributed one-dimensional stochastic processes supported on a filtered probability space, $(\Omega, \mathscr{F}, \mathscr{F}_t, \mathbb{P})$, such that each $X^{(i)}$ is a strong Markov process with respect to the filtration. Assume that $X_0^{(1)} < \cdots < X_0^{(N)}$. Suppose that $X_t^{(j)} \geq X_t^{(i)}$ for some $t > 0$ and $i < j$ implies that there is a time $\tau \leq t$ such that $X_\tau^{(i)} = X_\tau^{(j)}$. Then, for any collection of disjoint Borel subsets $A_1, \dots, A_N \subset \mathbb{R}$ such that $x \in A_i$, $y \in A_j$ and $i > j$ imply $x < y$,*

$$\begin{aligned} &\mathbb{P}(X_T^{(1)} \in A_1, \dots, X_T^{(N)} \in A_N; X_t^{(1)} < \cdots < X_t^{(N)} \text{ for all } t \in [0, T]) \\ &\quad = \det\big(P_T(X_0^{(i)}, A_j)\big)_{i,j=1}^N \end{aligned} \tag{5}$$

where $P_t(x, A)$ is the time t transition probability for the $X^{(i)}$ processes to move from x to A.

2 The Models

In this section we describe a selection of combinatorial and probabilistic models whose fluctuations are related to random matrix theory and whose analysis can be approached by considering non-intersecting random walk ensembles.

2.1 Longest Increasing Subsequence of a Random Permutation

The longest increasing subsequence problem can be formulated in the following manner. Denote by S_n the symmetric group on n symbols endowed with uniform measure. Given $\pi \in S_n$, a subsequence $\pi(i_1), \dots, \pi(i_r)$ is called an increasing subsequence if $i_1 < \cdots < i_r$ and $\pi(i_1) < \cdots < \pi(i_r)$. Denote by $\ell_n(\pi)$ the length of the longest increasing subsequence of π (this subsequence need not be unique). For applications of ℓ_n and problems related to the asymptotic behavior of ℓ_n see [1, 7, 21], for example. In particular, Baik, Deift, and Johansson [7] proved the following remarkable limit theorem:

$$\lim_{n\to\infty} \mathbb{P}\left(\frac{\ell_n(\pi) - 2\sqrt{n}}{n^{1/6}} < x\right) = F_{TW}(x). \tag{6}$$

A closely related object is the uniform measure on the set of pairs of standard Young tableaux having the same shape (equivalently, the so-called Plancherel measure on the set of partitions). Given a partition of n, $\lambda = (\lambda_1, \ldots, \lambda_r)$, where $\lambda_1 \geq \cdots \geq \lambda_r > 0$ and $\lambda_1 + \cdots + \lambda_r = n$, a standard Young tableaux of shape λ consists of r rows of boxes with distinct entries from $\{1, \ldots, n\}$ such that the rows are left-justified, the ith row has λ_i boxes, and the entries are constrained to increase along rows and columns from left to right and top to bottom, respectively. These objects will be called row increasing Young tableaux if the rows increase but the columns do not necessarily increase. The Robinson-Schensted bijection implies that the number of boxes in the top row of the pair of standard Young tableaux corresponding to $\pi \in S_n$ is equal to $\ell_n(\pi)$ [50]. Therefore, the distribution of ℓ_n is same as the distribution of the number of boxes in the top row of the pair of standard Young tableaux having the same shape chosen uniformly. This correspondence provides a representation of ℓ_n which is computable in terms of explicit formulae if the number of standard Young tableaux of a given shape is computable.

One way (among many) to compute the number of standard Young tableaux of shape λ is by employing a non-intersecting continuous time random walk argument [35]. Let $N_t^1, \ldots, N_t^r$ be independent rate 1 Poisson processes with initial conditions $N_0^i = 1 - i$ for $i = 1, 2, \ldots, r$. Define A_λ to be the event that $N_1^i = \lambda_i + (1 - i)$ for all $i = 1, 2, \ldots, r$. For almost every element of A_λ (the elements of A_λ where no two jumps of these processes occurs at the same time) there is a natural map to a row increasing Young tableaux. The map is defined as follows: If N^i jumps first then place a 1 in the leftmost box in row i; if N^j jumps second then place a 2 in the first box of row j if $j \neq i$ and a 2 in the second box of row i if $j = i$; continue in this fashion to produce a row increasing Young tableaux of shape λ. It is not hard to show that this map induces the uniform probability measure (when properly normalized by $\mathbb{P}(A_\lambda)$) on the row increasing Young tableaux. The subset $B_\lambda \subset A_\lambda$ which is mapped to the standard Young tableaux of shape λ corresponds to the realizations whose paths do not intersect each other for all $t \in [0, 1]$. Since the mapping described induces uniform measure on the row increasing Young tableaux of shape λ and the standard Young tableaux correspond to non-intersecting path realizations, B_λ, the number of standard Young tableaux of shape λ can be computed by evaluating:

$$|\text{row increasing Young tableaux of shape } \lambda| \frac{\mathbb{P}(B_\lambda)}{\mathbb{P}(A_\lambda)}. \tag{7}$$

The denominator of (7) is $e^{-r} \prod_{i=1}^r \frac{1}{\lambda_i!}$ by definition of Poisson processes and the independence of the N^i while $|\text{row increasing Young tableaux of shape } \lambda| = \frac{n!}{\lambda_1! \cdots \lambda_r!}$ by elementary combinatorics. On the other hand, via the Karlin-McGregor formula [36],

$$\mathbb{P}(B_\lambda) = \det\left(\frac{e^{-1}}{(\lambda_i - i + j)!} \right)_{i,j=1}^r. \tag{8}$$

Hence, the number of standard Young tableaux of shape λ is $n! \det(\frac{1}{(\lambda_i - i + j)!})_{i,j=1}^r$.

In tandem with the RSK correspondence this formula leads to an algebraic formula for the number of $\pi \in S_n$ for which $\ell_n(\pi) \leq m$. Moreover, a slight extension of this argument shows that the result (6) can be stated in terms of the top curve of the nonintersecting Poisson processes if these processes were forced to return to their initial locations at time 2 by imposing that their dynamics between times 1 and 2 have negative rather than positive jumps. The asymptotic behavior of other curves can also be studied [8, 44, 18, 32, 9]. Essentially, one can analyze the asymptotic behavior of ℓ_n by studying the fluctuations of the top path of a non-intersecting random walk ensemble. For related non-intersecting Poisson random walk ensembles, see for example [11, 38].

2.2 ABC-Hexagon

Kurt Johansson [34] discovered that random matrix theory is intimately related to several random tiling models. His analysis relied heavily on non-intersecting random walk technology applied to random tilings of both the Aztec diamond and the ABC-hexagon. We discuss the ABC-hexagon as the analysis fits more easily into the theory of non-intersecting Markov processes while the analysis of the Aztec diamond is more intimately connected to a graph theoretic presentation of the Karlin-McGregor formula.

Consider n symmetric simple random walks $S(m) = (S^{(1)}(m), \ldots, S^{(n)}(m))$, conditioned both not to intersect and to satisfy $S(0) = (2(n-1), 2(n-2), \ldots, 0) = S(2k)$. Any realization of such walks is in one-to-one correspondence to a rhombus tiling of a hexagon with sides of lengths k, k, n, k, k, n as Fig. 1 illustrates. Using the theorem of Karlin and McGregor, the distribution of $S(k)$ can be expressed in terms of a determinant. This determinant was significantly simplified and was shown to be related to the so-called Hahn orthogonal polynomials by Johansson [34]. In a tour de force, Baik, Kriecherbauer, McLaughlin, and Miller [10, 12] analyzed the asymptotic behavior of the Hahn polynomials and showed that as $n, k \to \infty$ in such a way that $k = O(n)$, the distribution of the top walker's position, $S^{(1)}(k)$, converges to F_{TW} and the gap distribution in the 'bulk' converges to a discrete version of F_{Sine}. A similar asymptotic result was obtained by Johansson [34] for random domino tilings of the Aztec diamond. Okounkov and Reshetikhin also considered a model closely related to the ABC-hexagon, see [45].

2.3 Last Passage Percolation

Consider the $\mathbb{N} \times \mathbb{N}$ lattice and a family of associated independent identically distributed random variables $\{X_i^j\}_{i,j=1}^{\infty}$. An *up/right path* π from the site $(1, 1)$ to the site (N, k) is a collection of sites $\{(i_k, j_k)\}_{k=1}^{N+k-1}$ satisfying $(i_1, j_1) = (1, 1)$, $(i_{N+k-1}, j_{N+k-1}) = (N, k)$, and $(i_{k+1}, j_{k+1}) - (i_k, j_k) \in \{(1, 0), (0, 1)\}$. Let

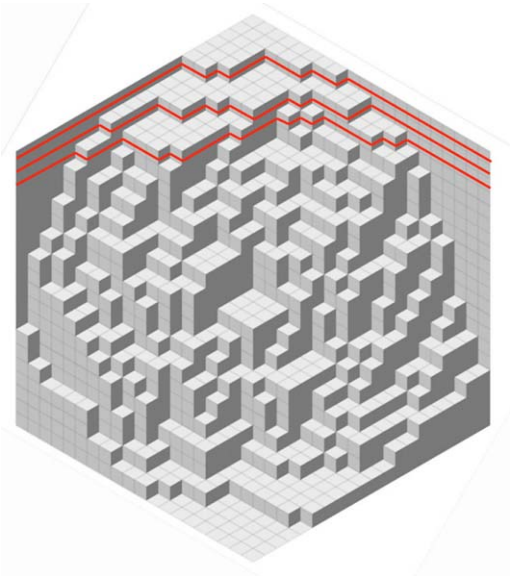

Fig. 1 Lozenge Tiling of the ABC-hexagon

$(1,1) \nearrow (N,k)$ denote the set of such up/right paths. The directed last passage time to $(N,k) \in \mathbb{N} \times \mathbb{N}$, denoted by $L(N,k)$, is defined by

$$L(N,k) = \max_{\pi \in (1,1) \nearrow (N,k)} \sum_{(i,j) \in \pi} X_i^j. \tag{9}$$

If X_i^j is interpreted as the time to pass the site $(i,\ j)$, $L(N,k)$ represents the maximal time to travel from the site $(1,\ 1)$ to (N,k) along an admissible path. It is interesting to note that the directed last passage percolation time can be viewed as a departure time in queuing theory (see e.g. [29]). In addition, directed last passage percolation is related to the flux of particles at a given site in the totally asymmetric simple exclusion process (see e.g. [48]).

Kurt Johansson [31] discovered that if the $\{X_i^j\}_{i,j=1}^{\infty}$ are independent identically distributed geometric random variables with parameter q then the probability distribution for the correctly normalized fluctuations of the last passage time, $L(N,k)$, is given by the Tracy-Widom distribution, F_{TW}. The precise statement of this remarkable fact is: For any $\rho \in (0,1]$,

$$\lim_{N \to \infty} \mathbb{P}\left(\frac{L(N, \lfloor \rho N \rfloor) - c_1(\rho,q)N}{c_2(\rho,q)N^{\frac{1}{3}}} \leq s \right) = F_{TW}(s), \tag{10}$$

where c_1 and c_2 are explicit constants depending only on ρ and q. By a limiting argument, Johansson was also able to prove this result in the case of exponential random variables [31].

In order to understand the connection between non-intersecting paths and last passage percolation, we briefly introduce a construction due to Neil O'Connell and Marc Yor [43, 42]. Let $D_0([0,\infty),\mathbb{R})$ be the Skorohod space of real valued right continuous functions with left hand limits subject to $f(0)=0$ and topologized with respect to the Skorohod metric. For $f, g \in D_0([0,\infty),\mathbb{R})$, define

$$f \otimes g(t) = \inf_{0\le s\le t}\big[f(s)+g(t)-g(s)\big], \tag{11}$$

$$f \odot g(t) = \sup_{0\le s\le t}\big[f(s)+g(t)-g(s)\big]. \tag{12}$$

In the present context, the order of operations is from left to right. Define a sequence of mappings $\Gamma_k : D_0([0,\infty),\mathbb{R})^k \to D_0([0,\infty),\mathbb{R})^k$ by

$$\Gamma_2(f,g) = (f\otimes g, g\odot f), \tag{13}$$

and for $k>2$,

$$\begin{aligned}\Gamma_k(f_1,\dots,f_k) = \big(&f_1\otimes f_2\otimes f_3\otimes\cdots\otimes f_k,\\ &\Gamma_{k-1}(f_2\odot f_1, f_3\odot(f_1\otimes f_2),\dots,\\ &\quad f_k\odot(f_1\otimes\cdots\otimes f_{k-1}))\big).\end{aligned} \tag{14}$$

O'Connell and Yor proved that if $B_1,\dots,B_k$ are independent standard one-dimensional Brownian motions, $\Gamma_k(B_1,\dots,B_k)$ is a Markov process with respect to its own filtration and has the same distribution on path space, $D_0([0,\infty),\mathbb{R})^k$, as k one-dimensional Brownian motions starting from the origin and conditioned (in the sense of Doob) never to collide. It is well known that this process can be interpreted as the k-dimensional GUE Dyson eigenvalue process. The first coordinate of Γ_k is the smallest eigenvalue, the second coordinate of Γ_k is the second smallest eigenvalue, and so on.

Fixing k, letting N tend to ∞, and employing Brownian scaling, it is not hard to see that last passage problem is intimately related to the non-intersecting path description of O'Connell and Yor. In particular, by considering the last passage problem with the random variables $\{Y_i^j\}$ where $Y_i^j = -X_i^j$, we see that the first coordinate of the Γ process is the last passage time. Under Brownian scaling, the Γ process converges to the GUE Dyson Brownian motion [43]. So, the last passage time for k fixed and $N\to\infty$ is given by the top eigenvalue of the k-dimensional Dyson Brownian motion, thus showing that the fluctuations of the last passage time are exactly the same as those of the top eigenvalue of the Gaussian Unitary Ensemble of $k\times k$ random matrices. Formally taking the limit as $k\to\infty$ explains, in a heuristic fashion, the appearance of F_{TW} in the last passage percolation problem. For another point of view on the last passage problem (which does not use non-intersecting paths), see [30, 13].

The universality conjecture in this context is a natural and unsolved problem. In particular, does the same fluctuation theorem hold for random variables other than geometric and exponential? We discuss further aspects of this question in Sect. 3.1.

2.4 Non-intersecting Brownian Motion

In this section we describe an example, due to Kurt Johansson [34], which connects non-intersecting Markov processes to random matrix theory in a finite n setting, i.e. no limit is involved. This example is also appealing from a probabilistic point of view in the same sense as Donsker's theorem for classical random walks: Non-intersecting path conditions provide a natural testing ground for central limit theorems with random matrix limiting distributions since one could imagine that non-intersecting Brownian motions are a natural limit of non-intersecting random walks.

Let $B_t = (B_t^{(1)}, \dots, B_t^{(n)})$ be an n-dimensional standard Brownian motion. We compute the density function of B_1 conditioned on the event that $B_t^{(1)} > B_t^{(2)} > \cdots > B_t^{(n)}$ for $0 < t < 2$ and $B_0 = B_2 = (0, \dots, 0)$. Let $p_t(x, y) = \frac{1}{\sqrt{2\pi t}} e^{-\frac{(x-y)^2}{2t}}$. The Karlin-McGregor formula [36] shows that the time t the density function of n one-dimensional non-intersecting Brownian motions with initial positions $(x_1, \dots, x_n)$, $x_1 > \cdots > x_n$, is given by

$$f_t(b_1, \dots, b_n) = \det(p_t(x_i, b_j))_{i,j=1}^n, \quad b_1 > \cdots > b_n. \tag{15}$$

Hence, the density function of B_1 for $b_1 > \cdots > b_n$ is equal to

$$\begin{aligned} f(b_1, \dots, b_n) &= \lim_{x,y \to 0} \frac{\det(p_1(x_i, b_j))_{i,j=1}^n \cdot \det(p_1(b_i, y_j))_{i,j=1}^n}{\det(p_2(x_i, y_j))_{i,j=1}^n} \\ &= \frac{2^{n(n-1)/2}}{\pi^{n/2} \prod_{j=1}^{n-1} j!} \prod_{1 \le i < j \le n} |b_i - b_j|^2 \prod_{j-1}^{n} e^{-b_j^2}. \end{aligned} \tag{16}$$

Equation (16) is precisely the eigenvalues density of an $n \times n$ random Hermitian matrix which has been chosen from the GUE. Well-known results of random matrix theory [53, 55] imply

$$\lim_{n \to \infty} \mathbb{P}\big((B_1^{(1)} - \sqrt{2n})\sqrt{2} n^{1/6} \le x\big) = F_{TW}(x). \tag{17}$$

In other words, the fluctuations of the top Brownian path are exactly described by the fluctuations of the top eigenvalue of a GUE random matrix, not only in the $n \to \infty$ limit but also at finite n. In Sect. 3.2 we discuss a non-intersecting random walk version of this model and issues related to universality with respect to the increments of the random walks. For other interesting non-intersecting Brownian motion processes, see for example [56, 16].

3 Universality

The notion of universality has played an important role in both mathematics and physics. For example, one of the basic theorems in classical probability theory is the central limit theorem which states that, when centered and scaled correctly, the distribution of a sum of independent identically distributed random variables with finite second moment converges to the Gaussian distribution. Universality has also played a prominent role in the development of many statistical mechanical models. Random matrix theory is no exception, see for example [22].

Before describing universality results in the context of last passage percolation and non-intersecting random walks we briefly mention two types of universality results in the context of random matrix theory. The first class of results pertain to universality of the Tracy-Widom and sine kernel distributions in the context of ensembles of random matrices whose distribution is invariant under unitary conjugation while the second pertains to universality of the Tracy-Widom and sine kernel distributions for the fluctuations of the top eigenvalue and the eigenvalue spacings of Wigner matrices.

Unitary Invariant Ensembles: Rather than considering the case of the GUE one can consider a random matrix ensemble equipped with the measure $e^{-TrV(H)}dH$ on Hermitian matrices where V is a function which tends to ∞ at both $\pm\infty$ and satisfies one of a variety of technical conditions. In this case, the goal is to prove universality of the fluctuations of the top eigenvalue and gap probabilities in the bulk. Obtaining such universality results, even when dealing with explicit correlation functions/gap probabilities, is not trivial and requires new non-classical methods, see [25–27, 46, 15, 23, 40]. However, under the correct scaling and centering, the top eigenvalue does indeed display Tracy-Widom fluctuations and the fluctuations in the bulk are described by the sine kernel, thus providing a variety of important cases in which universality of the Tracy-Widom and sine kernel distribution can be proven.

Wigner Matrices: Wigner matrices also display universality of the Tracy-Widom distribution for the fluctuations of the top eigenvalue [49]. In particular, Soshnikov [49] proved that the fluctuations of the properly scaled and centered top eigenvalue are given by the GUE Tracy-Widom law for any ensemble of Hermitian matrices with independent identically distributed entries subject to the Hermitian condition and several technical assumptions. S. Péché and A. Soshnikov [47] have recently made further progress in this direction. Johansson proved a universality result in the bulk for a special class of Wigner matrices [33]. G. BenArous and S. Péché [14] proved an analogous result in the case of sample covariance matrices. However, the general universality conjecture in the bulk, if true, remains an important open problem.

In the next two subsections we describe results which hint at universality of the Tracy-Widom and sine kernel distributions in the case of last passage percolation and non-intersecting walks.

3.1 Last Passage Percolation

The fluctuations of the last passage percolation time in the case of general random variables is interesting from the probabilistic point of view and pertains to the question of universality of the Tracy-Widom distribution in a non-exactly solvable setting, i.e. there are no known algebraically tractable formulae which describe the distribution of the last passage time for finite size rectangles.

However, universality can be proven if the lengths of the sides of the rectangles do not grow linearly with respect to each other. In particular, Jinho Baik and the author [5] and independently Thierry Bodineau and James Martin [17] proved that universality holds in thin rectangles. One version of the main result of these investigations follows.

Theorem 2 ([17], see also [5] when $p = 4$). *Suppose that $\{X_i^j\}_{i,j=1}^{\infty}$ is a family of independent identically distributed random variables such that $\mathbb{E}X_i^j = \mu$, $\mathbb{E}|X_i^j|^2 - \mu^2 = \sigma^2$, and $\mathbb{E}|X_i^j|^p < \infty$ for some $p > 2$. For any $x \in \mathbb{R}$,*

$$\lim_{N,k\to\infty} \mathbb{P}\left(\frac{L(N,k) - \mu(N+k-1) - 2\sigma\sqrt{Nk}}{\sigma k^{-1/6} N^{\frac{1}{2}}} \leq x \right) = F_{TW}(x), \tag{18}$$

where $k = o(N^{\alpha})$ and $\alpha < \frac{6}{7}(\frac{1}{2} - \frac{1}{p})$.

This states that the Tracy-Widom distribution is indeed universal, at least in some scaling regimes, in the case of last passage percolation. The proof of this result uses strong approximation techniques which couple random walks to Brownian motion. For the case $\mathbb{E}|X_i^j|^3 < \infty$ the present author [52] proved the above result using a different technique which relies on the ideas of S. Chatterjee [19] in the spirit of Lindeberg's proof of the central limit theorem. It is interesting that, in the case $p = 3$, both techniques break down at the scaling $\alpha = \frac{1}{7}$.

These techniques do not effectively lead to analysis of the regime in which k and N grow linearly with respect to each other. This scaling is the most interesting and presents a challenge.

3.2 Non-intersecting Random Walks

As already noted, many models which give rise to random matrix fluctuations can be formulated in terms of non-intersecting random walks. With this in mind, Jinho Baik and the author [6] considered ensembles of non-intersecting random walks with general increments with the hope of understanding the robustness of the Tracy-Widom and sine kernel distributions in the context of general non-intersecting random walks. This section describes the results of that investigation.

Let k be a positive integer. Let

$$x_i = \frac{2i-k}{k}, \quad i \in \{0, \ldots, k\}. \tag{19}$$

Note that $x_i \in [-1, 1]$ for all i. Let $\{Y_l^j\}_{j=0,l=1}^{k,N_k}$ be a family of independent identically distributed random variables where N_k is a positive integer. Assume that $\mathbb{E}Y_l^j = 0$ and $Var(Y_l^j) = 1$. Further assume that there is $\lambda_0 > 0$ such that $\mathbb{E}(e^{\lambda Y_l^j}) < \infty$ for all $|\lambda| < \lambda_0$.

Define the random walk process $S(t) = (S_0(t), \ldots, S_k(t))$ by

$$S_j(t) = x_j + \sqrt{\frac{2}{N_k}}\left(\sum_{i=1}^{\lfloor \frac{tN_k}{2} \rfloor} Y_i^j + \left(\frac{tN_k}{2} - \left\lfloor \frac{tN_k}{2} \right\rfloor\right) Y^j_{\lfloor \frac{tN_k}{2} \rfloor + 1}\right), \quad \text{for } t \in [0, 2]. \tag{20}$$

For N_k equally spaced times, S_j is given by

$$S_j\left(\frac{2}{N_k}l\right) = x_j + \sqrt{\frac{2}{N_k}}(Y_1^j + \cdots + Y_l^j), \quad l = 1, 2, \ldots, N_k. \tag{21}$$

For t between $\frac{2}{N_k}l$ and $\frac{2}{N_k}(l+1)$, $S_j(t)$ is simply defined by linear interpolation.

Let $(C([0, 2]; \mathbb{R}^{k+1}), \mathscr{C})$ be the family of measurable spaces constructed from the continuous functions on $[0, 2]$ taking values in $\mathbb{R}^{k+1}$ equipped with their Borel sigma algebras (generated by the sup norm). Let $A_k, B_k \in \mathscr{C}$ be the events defined by

$$A_k = \{y_0(t) < \cdots < y_k(t) \text{ for } t \in [0, 2]\}, \tag{22}$$

$$B_k = \{y_i(2) \in [x_i - h_k, x_i + h_k] \text{ for } i \in \{0, \ldots, k\}\} \tag{23}$$

where $h_k > 0$. The results described below concerns the $S(t)$ process conditioned on the event $A_k \cap B_k$ where $h_k \ll \frac{2}{k}$. In other words, the particles never intersect and all particles essentially return to their original location at the final time $t = 2$.

Under technical conditions on h_k and N_k, as $k \to \infty$, the limiting fluctuations of the locations of the particles at time $t = 1$, after suitable scaling, are given by the Tracy-Widom and sine kernel distributions at the edge and in the bulk, respectively. The conditions for h_k and N_k are that $\{h_k\}_{k>0}$ is a sequence of positive numbers and $\{N_k\}_{k>0}$ is a sequence of positive integers satisfying

$$h_k \le (2k)^{-2k^2} \quad \text{and} \quad N_k \ge h_k^{-4(k+2)}. \tag{24}$$

Let $C_k, D_k \in \mathscr{C}$ be defined by

$$C_k = \left\{y_k(1) \le \sqrt{2k} + \frac{\xi}{\sqrt{2}k^{1/6}}\right\}, \tag{25}$$

$$D_k = \left\{y_i(1) \notin \left[-\frac{\pi\eta}{\sqrt{2k}}, \frac{\pi\eta}{\sqrt{2k}}\right] \text{ for all } i \in \{0, \ldots, k\}\right\}, \tag{26}$$

where ξ and $\eta > 0$ are fixed real numbers. The event C_k is a constraint on the location of the right-most particle, and D_k is the event that no particle is in a small neighborhood of the origin at time 1.

Theorem 3. *Let $\mathbb{P}^{(k)}$ be the probability measure induced on $(C([0,2];\mathbb{R}^{k+1}),\mathscr{C})$ by the random walks $\{S(t) : t \in [0,2]\}$. Let $\{h_k\}_{k>0}$ and $\{N_k\}_{k>0}$ satisfy (24). Then*

$$\lim_{k\to\infty} \mathbb{P}^{(k)}(C_k | A_k \cap B_k) = F_{TW}(\xi). \tag{27}$$

A similar theorem holds for the bulk.

Theorem 4. *Let $\mathbb{P}^{(k)}$ be the probability measure induced on $(C([0,2];\mathbb{R}^{k+1}),\mathscr{C})$ by the random walks $\{S(t) : t \in [0,2]\}$, and let $\{h_k\}_{k>0}$ and $\{N_k\}_{k>0}$ satisfy (24). Then*

$$\lim_{k\to\infty} \mathbb{P}_k(D_k | A_k \cap B_k) = F_{Sine}(\eta). \tag{28}$$

These results are derived from strong approximation theorems and the Deift-Zhou steepest descent method applied to Stieljes-Wigert polynomials. It would be interesting to know the full range of scalings of k, N_k for which the above theorems hold.

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Homogenization of Periodic Differential Operators as a Spectral Threshold Effect

Mikhail S. Birman and Tatiana A. Suslina

Abstract The present paper is devoted to the homogenization problem for a wide class of periodic second order differential operators (DO's) in $\mathbb{R}^d$. This class includes a number of classical DO's of mathematical physics. We propose a brief survey of the results obtained in a series of Birman and Suslina (Systems, Approximations, Singular Integral Operators and Related Topics, Oper. Theory Adv. Appl., vol. 129, pp. 71–107, 2001; Algebra Anal. 15(5):108, 2003; Algebra Anal. 17(5):69–90, 2005; Algebra Anal. 17(6):1–104, 2005; Algebra Anal. 18(6):1–130, 2006).

1 Introduction

The present paper is devoted to the homogenization problem for a wide class of periodic second order differential operators (DO's) in $\mathbb{R}^d$. This class includes a number of classical DO's of mathematical physics. We propose a brief survey of the results obtained in a series of papers [2, 3, 5–7]. In these papers, for the first time, convergence in the small period limit (as $\varepsilon \to 0$) for the resolvent of the operator family to the resolvent of the *homogenized operator* with sharp-order error estimate in the *operator norm* is established.

By $L_2(\mathbb{R}^d; \mathbb{C}^n)$ we denote the L_2-space of $\mathbb{C}^n$-valued functions in $\mathbb{R}^d$; and by $H^1(\mathbb{R}^d; \mathbb{C}^n)$ we denote the Sobolev class of first order. Let $\mathcal{A}$ be a matrix elliptic second order DO acting in $L_2(\mathbb{R}^d; \mathbb{C}^n)$ and given by the differential expression $\mathcal{A}(\mathbf{x}, \mathbf{D})$, $\mathbf{x} \in \mathbb{R}^d$, $\mathbf{D} = -i\nabla$. Suppose that coefficients of $\mathcal{A}(\mathbf{x}, \mathbf{D})$ are periodic with respect to some lattice $\Gamma \subset \mathbb{R}^d$. By Ω we denote the elementary cell of the lattice

Mikhail S. Birman
Faculty of Physics, St. Petersburg State University, Ulyanovskaya, 3, St. Petersburg 198504, Russian Federation

Tatiana A. Suslina
Faculty of Physics, St. Petersburg State University, Ulyanovskaya, 3, St. Petersburg 198504, Russian Federation, e-mail: suslina@list.ru

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Γ; $\widetilde{\Gamma}$ is the lattice dual to Γ, and $\widetilde{\Omega}$ stands for the central Brillouin zone of $\widetilde{\Gamma}$. (For instance, if $\Gamma = \mathbb{Z}^d$, then $\Omega = (0, 1)^d$; $\widetilde{\Gamma} = (2\pi\mathbb{Z})^d$ and $\widetilde{\Omega} = (-\pi, \pi)^d$.) The precise definition of DO $\mathcal{A}$ is given in Sect. 2; see (5), (6). The operator $\mathcal{A}$ is selfadjoint and non-negative, the bottom of its spectrum is the point $\lambda = 0$.

Along with $\mathcal{A}$, we consider the family of operators $\mathcal{A}_\varepsilon$ given by the expression $\mathcal{A}(\mathbf{x}/\varepsilon, \mathbf{D})$ with rapidly oscillating (as $\varepsilon \to 0$) coefficients. Our goal is to *describe the behavior of the resolvent* $(\mathcal{A}_\varepsilon + I)^{-1}$ *as* $\varepsilon \to 0$. In [2, 3, 5–7], new results in the homogenization theory are obtained. Namely, we find approximation for the resolvent $(\mathcal{A}_\varepsilon + I)^{-1}$ in the operator norm in $L_2(\mathbb{R}^d; \mathbb{C}^n)$ in terms of the resolvent of the effective operator with sharp-order remainder estimate (by $C\varepsilon$). Besides, we obtain more accurate approximation for the resolvent in the $L_2(\mathbb{R}^d; \mathbb{C}^n)$-operator norm with the error term of order ε^2 and also approximation for the resolvent in the operator norm from $L_2(\mathbb{R}^d; \mathbb{C}^n)$ to $H^1(\mathbb{R}^d; \mathbb{C}^n)$ with error of order ε. In such approximations, besides the principal term, we have to take into account terms of order ε (the so called *corrector*). Herewith, it turns out that the form of the corrector depends on the type of operator norm in approximation.

The method of investigation is described in Sect. 6. Now we only give some comments on the simplest Theorem 1. Periodicity of the operator $\hat{\mathcal{A}}$ of the form (6) allows us to apply the Floquet-Bloch decomposition (see relation (32)). Next, let T_ε be the (unitary) scale transformation: $(T_\varepsilon \mathbf{u})(\mathbf{x}) = \varepsilon^{d/2}\mathbf{u}(\varepsilon\mathbf{x})$. Then

$$(\hat{\mathcal{A}}_\varepsilon + I)^{-1} = \varepsilon^2 T_\varepsilon^* (\hat{\mathcal{A}} + \varepsilon^2 I)^{-1} T_\varepsilon. \tag{1}$$

The identity (1) shows that, in essential, the problem is reduced to the study of the resolvent $(\hat{\mathcal{A}} + \varepsilon^2 I)^{-1}$. Therefore, it turns out that the homogenization effect is closely related to the behavior of the resolvent of $\hat{\mathcal{A}}$ near the bottom of its spectrum $\lambda = 0$. That is why the homogenization procedure can be treated as a *spectral threshold effect*. We prove that the resolvent $(\hat{\mathcal{A}} + \varepsilon^2 I)^{-1}$ can be approximated in terms of the resolvent of the effective operator $\hat{\mathcal{A}}^0$ with constant coefficients (see (39)). Since T_ε is unitary operator, (1) and (39) imply the main estimate (11).

It must be mentioned that the Floquet-Bloch decomposition was employed for the study of homogenization problems before (see, e. g., [10, 18, 9], where the scalar elliptic operator $-\operatorname{div} g(\mathbf{x})\nabla$ was considered). However, the question about estimates of the form (11) has not been even asked. Some weaker types of convergence were studied; then relations of the form (1) are useless, since the behavior of T_ε as $\varepsilon \to 0$ is non-controlled.

2 Periodic DO's. The Effective Matrix

We distinguish a wide class of second order matrix periodic DO's acting in $L_2(\mathbb{R}^d; \mathbb{C}^n)$. Let $m \geq n$, and let $\mathcal{X} : L_2(\mathbb{R}^d; \mathbb{C}^n) \to L_2(\mathbb{R}^d; \mathbb{C}^m)$ be a homogeneous first order DO of the form $\mathcal{X} = h(\mathbf{x})b(\mathbf{D})f(\mathbf{x})$. Here an $(m \times m)$-matrix-valued function $h(\mathbf{x})$ and an $(n \times n)$-matrix-valued function $f(\mathbf{x})$ are Γ-periodic

and bounded together with the inverse matrices:

$$h, h^{-1} \in L_\infty; \quad f, f^{-1} \in L_\infty. \tag{2}$$

Next, $b(\mathbf{D})$ is a homogeneous first order DO with constant coefficients; its symbol $b(\boldsymbol{\xi})$ is an $(m \times n)$-matrix-valued linear homogeneous function of $\boldsymbol{\xi} \in \mathbb{R}^d$. We assume that $\operatorname{rank} b(\boldsymbol{\xi}) = n$, $\boldsymbol{\xi} \neq 0$. Then

$$\alpha_0 \mathbf{1}_n \leq b(\boldsymbol{\theta})^* b(\boldsymbol{\theta}) \leq \alpha_1 \mathbf{1}_n, \quad |\boldsymbol{\theta}| = 1, \quad 0 < \alpha_0 \leq \alpha_1 < \infty, \tag{3}$$

for some constants α_0, α_1. (By $\mathbf{1}_n$ we denote the unit $(n \times n)$-matrix.) Under conditions (2) and (3), the operator $\mathcal{X}$ is closed on the domain $\operatorname{Dom} \mathcal{X} = \{\mathbf{u} \in L_2(\mathbb{R}^d; \mathbb{C}^n) : f\mathbf{u} \in H^1(\mathbb{R}^d; \mathbb{C}^n)\}$.

Our main object is the selfadjoint operator $\mathcal{A} = \mathcal{X}^* \mathcal{X}$ in $L_2(\mathbb{R}^d; \mathbb{C}^n)$. The operator $\mathcal{A}$ is generated by the closed quadratic form

$$a[\mathbf{u}, \mathbf{u}] = \int_{\mathbb{R}^d} |h(\mathbf{x}) b(\mathbf{D}) f(\mathbf{x}) \mathbf{u}|^2 \, d\mathbf{x}, \quad \mathbf{u} \in \operatorname{Dom} \mathcal{X}.$$

Conditions (2) and (3) imply that

$$c_0 \int_{\mathbb{R}^d} |\mathbf{D}(f\mathbf{u})|^2 \, d\mathbf{x} \leq a[\mathbf{u}, \mathbf{u}] \leq c_1 \int_{\mathbb{R}^d} |\mathbf{D}(f\mathbf{u})|^2 \, d\mathbf{x}, \quad \mathbf{u} \in \operatorname{Dom} \mathcal{X},$$

$$c_0 = \alpha_0 \|h^{-1}\|_{L_\infty}^{-2}, \quad c_1 = \alpha_1 \|h\|_{L_\infty}^2. \tag{4}$$

Formally, $\mathcal{A}$ corresponds to the differential expression

$$\mathcal{A} = \mathcal{A}(g, f) = f(\mathbf{x})^* b(\mathbf{D})^* g(\mathbf{x}) b(\mathbf{D}) f(\mathbf{x}), \quad g(\mathbf{x}) := h(\mathbf{x})^* h(\mathbf{x}). \tag{5}$$

In the case where $f = \mathbf{1}_n$, we use the notation

$$\hat{\mathcal{A}} = \hat{\mathcal{A}}(g) = b(\mathbf{D})^* g(\mathbf{x}) b(\mathbf{D}). \tag{6}$$

Many operators of mathematical physics admit such factorization. The acoustics operator and the operator of elasticity theory have the form (6). The Schrödinger operator and the two-dimensional Pauli operator can be written in the form (5) with $f \neq \mathbf{1}_n$.

By $\widetilde{H}^1(\Omega; \mathbb{C}^n)$ we denote the subspace of functions in $H^1(\Omega; \mathbb{C}^n)$, whose Γ-periodic extension to $\mathbb{R}^d$ belongs to $H^1_{\mathrm{loc}}(\mathbb{R}^d; \mathbb{C}^n)$. Let $\mathbf{e}_1, \ldots, \mathbf{e}_m$ be the standard orthonormal basis in $\mathbb{C}^m$. Let $\mathbf{v}_j \in \widetilde{H}^1(\Omega; \mathbb{C}^n)$ be the (weak) periodic solution of the following problem on the cell Ω:

$$b(\mathbf{D})^* g(\mathbf{x}) (b(\mathbf{D}) \mathbf{v}_j(\mathbf{x}) + \mathbf{e}_j) = 0, \qquad \int_\Omega \mathbf{v}_j(\mathbf{x}) \, d\mathbf{x} = 0, \quad j = 1, \ldots, m.$$

By $\Lambda(\mathbf{x})$ we denote the $(n \times m)$-matrix with the columns $\mathbf{v}_j(\mathbf{x})$. We put

$$\widetilde{g}(\mathbf{x}) = g(\mathbf{x})(b(\mathbf{D})\Lambda(\mathbf{x}) + \mathbf{1}_m), \tag{7}$$
$$g^0 = |\Omega|^{-1} \int_\Omega \widetilde{g}(\mathbf{x})\, d\mathbf{x}.$$

It turns out that the constant $(m \times m)$-matrix g^0 is positive. It is called the *effective matrix*. This matrix satisfies the estimates $\underline{g} \le g^0 \le \overline{g}$, where

$$\overline{g} = |\Omega|^{-1} \int_\Omega g(\mathbf{x})\, d\mathbf{x}, \quad \underline{g}^{-1} = |\Omega|^{-1} \int_\Omega g(\mathbf{x})^{-1}\, d\mathbf{x}.$$

These estimates are well known in the homogenization theory for particular DO's (the Voight-Reuss bracketing). It is interesting that, if $m = n$, then $g^0 = \underline{g}$ (see [3, Chap. 3, Theorem 1.5]). In particular, this is always true for the two-dimensional Pauli operator.

The operator

$$\hat{\mathcal{A}}^0 = b(\mathbf{D})^* g^0 b(\mathbf{D}) \tag{8}$$

with constant coefficients is called the *effective operator* for the operator (6).

3 Homogenization of Periodic DO's. Principal Term of Approximation for the Resolvent

Let $\varepsilon > 0$ be a parameter. For any Γ-periodic function ϕ we denote: $\phi^\varepsilon(\mathbf{x}) = \phi(\varepsilon^{-1}\mathbf{x})$. We consider the following operators

$$\hat{\mathcal{A}}_\varepsilon = \hat{\mathcal{A}}(g^\varepsilon) = b(\mathbf{D})^* g^\varepsilon b(\mathbf{D}), \tag{9}$$
$$\mathcal{A}_\varepsilon = \mathcal{A}(g^\varepsilon, f^\varepsilon) = (f^\varepsilon)^* b(\mathbf{D})^* g^\varepsilon b(\mathbf{D}) f^\varepsilon \tag{10}$$

with rapidly oscillating (as $\varepsilon \to 0$) coefficients. *Our goal is to approximate the resolvents* $(\hat{\mathcal{A}}_\varepsilon + I)^{-1}$, $(\mathcal{A}_\varepsilon + I)^{-1}$ *for small* $\varepsilon > 0$. We start with the principal term of approximation in the operator norm in $L_2(\mathbb{R}^d; \mathbb{C}^n)$.

Theorem 1. *Let* $\hat{\mathcal{A}}_\varepsilon$ *be the operator* (9)*, and let* $\hat{\mathcal{A}}^0$ *be the effective operator* (8)*. Then*

$$\|(\hat{\mathcal{A}}_\varepsilon + I)^{-1} - (\hat{\mathcal{A}}^0 + I)^{-1}\|_{L_2 \to L_2} \le C_1 \varepsilon, \quad 0 < \varepsilon \le 1. \tag{11}$$

The constant C_1 *depends only on the norms* $\|g\|_{L_\infty}$, $\|g^{-1}\|_{L_\infty}$, *on constants* α_0, α_1 *from* (3)*, and on parameters of the lattice* Γ.

If $f \ne \mathbf{1}$, it is impossible to find operator with constant coefficients such that its resolvent is the limit of the resolvent of $\mathcal{A}_\varepsilon$. However, it is possible *to approximate* $(\mathcal{A}_\varepsilon + I)^{-1}$ *in terms of the "generalized" resolvent of the operator* $\hat{\mathcal{A}}^0$*, sandwiched by rapidly oscillating coefficients.*

Theorem 2. *Let $\mathcal{A}_\varepsilon$ be the operator (10), and let $\hat{\mathcal{A}}^0$ be the operator (8). We put*

$$Q(\mathbf{x}) = (f(\mathbf{x}) f(\mathbf{x})^*)^{-1}, \quad \overline{Q} = |\Omega|^{-1} \int_\Omega Q(\mathbf{x})\, d\mathbf{x}. \tag{12}$$

Then we have

$$\|(\mathcal{A}_\varepsilon + I)^{-1} - (f^\varepsilon)^{-1}(\hat{\mathcal{A}}^0 + \overline{Q})^{-1}((f^\varepsilon)^*)^{-1}\|_{L_2 \to L_2} \le C_1^{(Q)}\varepsilon, \quad 0 < \varepsilon \le 1. \tag{13}$$

The constant $C_1^{(Q)}$ depends only on the norms $\|g\|_{L_\infty}$, $\|g^{-1}\|_{L_\infty}$, $\|f\|_{L_\infty}$, $\|f^{-1}\|_{L_\infty}$, on constants α_0, α_1, and on parameters of the lattice Γ.

Though the approximating operator in (13) contains rapidly oscillating coefficients, the inverse is taken only for operator with constant coefficients.

Estimates (11) are (13) are order-sharp, and constants in estimates are controlled explicitly. For the first time, Theorem 1 was established in [2], and Theorem 2 was proved in [3].

4 More Accurate Approximation for the Resolvent in the L_2-Operator Norm

In order to obtain more accurate approximations, we should take terms of order ε (the so called "corrector") into account. We start with the result for the operator (9).

Theorem 3. *Let $\hat{\mathcal{A}}_\varepsilon$ be the operator (9), and let $\hat{\mathcal{A}}^0$ be the effective operator (8). We have*

$$\|(\hat{\mathcal{A}}_\varepsilon + I)^{-1} - \left((\hat{\mathcal{A}}^0 + I)^{-1} + \varepsilon K(\varepsilon)\right)\|_{L_2 \to L_2} \le C_2 \varepsilon^2, \quad 0 < \varepsilon \le 1. \tag{14}$$

Here the corrector $K(\varepsilon)$ is the sum of three terms:

$$K(\varepsilon) = K_1(\varepsilon) + K_1(\varepsilon)^* + K_3. \tag{15}$$

The operator

$$K_1(\varepsilon) = \Lambda^\varepsilon \Pi_\varepsilon b(\mathbf{D})(\hat{\mathcal{A}}^0 + I)^{-1} \tag{16}$$

contains the rapidly oscillating matrix Λ^ε and also the smoothing operator Π_ε given by

$$(\Pi_\varepsilon \mathbf{u})(\mathbf{x}) = (2\pi)^{-d/2} \int_{\widetilde{\Omega}/\varepsilon} e^{i\langle \mathbf{x}, \boldsymbol{\xi}\rangle} \hat{\mathbf{u}}(\boldsymbol{\xi})\, d\boldsymbol{\xi}. \tag{17}$$

Here $\hat{\mathbf{u}}(\boldsymbol{\xi})$ is the Fourier image of $\mathbf{u}(\mathbf{x})$. The operator K_3 does not depend on ε. It is selfadjoint pseudodifferential operator of order (-1) given by

$$K_3 = -(\hat{\mathcal{A}}^0 + I)^{-1} b(\mathbf{D})^* L(\mathbf{D}) b(\mathbf{D})(\hat{\mathcal{A}}^0 + I)^{-1},$$

where $L(\mathbf{D})$ is the first order DO with the symbol

$$L(\boldsymbol{\xi}) = |\Omega|^{-1} \int_{\Omega} (\Lambda(\mathbf{x})^* b(\boldsymbol{\xi})^* \widetilde{g}(\mathbf{x}) + \widetilde{g}(\mathbf{x})^* b(\boldsymbol{\xi}) \Lambda(\mathbf{x})) \, d\mathbf{x}.$$

The constant C_2 in (14) depends only on the norms $\|g\|_{L_\infty}$, $\|g^{-1}\|_{L_\infty}$, on α_0, α_1, and on parameters of the lattice Γ. In expression (16) for $K_1(\varepsilon)$ the smoothing operator Π_ε can be replaced by I in the following cases: (a) *$d \le 4$,* (b) *for the scalar operator $\hat{\mathcal{A}} = \mathbf{D}^* g(\mathbf{x}) \mathbf{D}$, where $g(\mathbf{x})$ has real entries (d is arbitrary),* (c) *in the case where $g^0 = \underline{g}$ (d is arbitrary); in particular, if $m = n$. Under such replacement, only the constant C_2 will change.*

Note that the traditional corrector used in the homogenization theory differs from the term $K_1(\varepsilon)$ only by the absence of the operator Π_ε. The term K_3 has not been known before.

In certain sense, the third term of the corrector is the most important. The weak operator limit as $\varepsilon \to 0$ for first two terms is equal to zero (because of the presence of the rapidly oscillating factor Λ^ε with zero mean value). Therefore, $(w)\text{-}\lim_{\varepsilon \to 0} K(\varepsilon) = K_3$. In some cases $K_3 = 0$. In particular, this is true for the scalar operator $\mathbf{D}^* g(\mathbf{x}) \mathbf{D}$, where $g(\mathbf{x})$ has real entries. However, in general case K_3 is non-trivial, which is confirmed by examples for the scalar operator with complex-valued coefficients and also for matrix operators with real-valued coefficients.

The similar result is obtained for general operators $\mathcal{A}_\varepsilon$, but approximation contains rapidly oscillating factors.

Theorem 4. *Let $\mathcal{A}_\varepsilon$ be the operator (10), and let $\hat{\mathcal{A}}^0$ be the operator (8). Suppose that $Q(\mathbf{x})$ and $\overline{Q}$ are defined by (12). For $0 < \varepsilon \le 1$ we have*

$$\|(\mathcal{A}_\varepsilon + I)^{-1} - (f^\varepsilon)^{-1} \left((\hat{\mathcal{A}}^0 + \overline{Q})^{-1} + \varepsilon K^{(Q)}(\varepsilon) \right) ((f^\varepsilon)^*)^{-1} \|_{L_2 \to L_2} \le C_2^{(Q)} \varepsilon^2. \tag{18}$$

Here

$$\begin{aligned} K^{(Q)}(\varepsilon) &= K_1^{(Q)}(\varepsilon) + (K_1^{(Q)}(\varepsilon))^* + K_3^{(Q)}, \\ K_1^{(Q)}(\varepsilon) &= \Lambda^\varepsilon \Pi_\varepsilon b(\mathbf{D}) (\hat{\mathcal{A}}^0 + \overline{Q})^{-1}, \\ K_3^{(Q)} &= -\mathcal{R}_Q^0 \left(b(\mathbf{D})^* L(\mathbf{D}) b(\mathbf{D}) + b(\mathbf{D})^* (\overline{Q\Lambda})^* + (\overline{Q\Lambda}) b(\mathbf{D}) \right) \mathcal{R}_Q^0, \end{aligned} \tag{19}$$

$\mathcal{R}_Q^0 := (\hat{\mathcal{A}}^0 + \overline{Q})^{-1}$, and $\overline{Q\Lambda}$ is the mean value of the matrix-valued function $Q(\mathbf{x})\Lambda(\mathbf{x})$ over the cell Ω. The constant $C_2^{(Q)}$ in (18) depends only on the norms $\|g\|_{L_\infty}$, $\|g^{-1}\|_{L_\infty}$, $\|f\|_{L_\infty}$, $\|f^{-1}\|_{L_\infty}$, on α_0, α_1, and on parameters of the lattice Γ. In the expression for $K_1^{(Q)}(\varepsilon)$ the smoothing operator Π_ε can be replaced by I in the same cases as in Theorem 3.

Theorems 3 and 4 have been proved in [6].

5 ($L_2 \to H^1$)-Approximation of the Resolvent. Approximation of the Fluxes in L_2

In order to approximate the resolvent in the operator norm from $L_2(\mathbb{R}^d;\mathbb{C}^n)$ to $H^1(\mathbb{R}^d;\mathbb{C}^n)$ with the error $O(\varepsilon)$, it suffices to take into account only the first term $K_1(\varepsilon)$ of the corrector (15).

Theorem 5. *Let $\hat{\mathcal{A}}_\varepsilon$ be the operator (9), and let $\hat{\mathcal{A}}^0$ be the effective operator (8). Let $K_1(\varepsilon)$ be the operator (16). Then we have*

$$\|(\hat{\mathcal{A}}_\varepsilon + I)^{-1} - \left((\hat{\mathcal{A}}^0 + I)^{-1} + \varepsilon K_1(\varepsilon)\right)\|_{L_2\to H^1} \le C_3\varepsilon, \quad 0 < \varepsilon \le 1. \tag{20}$$

The constant C_3 in (20) depends only on the norms $\|g\|_{L_\infty}$, $\|g^{-1}\|_{L_\infty}$, on α_0, α_1, and on parameters of the lattice Γ. In the expression for $K_1(\varepsilon)$, the smoothing operator Π_ε can be replaced by I in the following cases: (a) *$d \le 2$,* (b) *for the scalar operator $\hat{\mathcal{A}} = \mathbf{D}^* g(\mathbf{x})\mathbf{D}$, where $g(\mathbf{x})$ has real entries (d is arbitrary),* (c) *if $g^0 = \underline{g}$ (in particular, if $m = n$).*

For the operator $\mathcal{A}_\varepsilon$ of the form (10) we obtain the following result.

Theorem 6. *Let $\mathcal{A}_\varepsilon$ be the operator (10), and let $\hat{\mathcal{A}}^0$ be the operator (8). Suppose that $\overline{Q}$ is defined by (12) and that $K_1^{(Q)}(\varepsilon)$ is the operator (19). Then for $0 < \varepsilon \le 1$ we have*

$$\|f^\varepsilon(\mathcal{A}_\varepsilon + I)^{-1} - \left((\hat{\mathcal{A}}^0 + \overline{Q})^{-1} + \varepsilon K_1^{(Q)}(\varepsilon)\right)((f^\varepsilon)^*)^{-1}\|_{L_2\to H^1} \le C_3^{(Q)}\varepsilon. \tag{21}$$

The constant $C_3^{(Q)}$ in (21) depends only on the norms $\|g\|_{L_\infty}$, $\|g^{-1}\|_{L_\infty}$, $\|f\|_{L_\infty}$, $\|f^{-1}\|_{L_\infty}$, on α_0, α_1, and on parameters of the lattice Γ. In the expression for $K_1^{(Q)}(\varepsilon)$ the smoothing operator Π_ε can be replaced by I in the same cases as in Theorem 5.

Theorems 5 and 6 have been proved in [7].

The results can be reformulated in terms of solutions. Let $\mathbf{u}_\varepsilon$ be the solution of the equation

$$\hat{\mathcal{A}}_\varepsilon \mathbf{u}_\varepsilon + \mathbf{u}_\varepsilon = \mathbf{F}, \quad \mathbf{F} \in L_2(\mathbb{R}^d;\mathbb{C}^n), \tag{22}$$

and let $\mathbf{u}_0$ be the solution of the "homogenized" equation

$$\hat{\mathcal{A}}^0 \mathbf{u}_0 + \mathbf{u}_0 = \mathbf{F}. \tag{23}$$

Then inequalities (11) and (20) mean that

$$\begin{aligned} &\|\mathbf{u}_\varepsilon - \mathbf{u}_0\|_{L_2} \le C_1\varepsilon\|\mathbf{F}\|_{L_2}, \quad 0 < \varepsilon \le 1, \\ &\|\mathbf{u}_\varepsilon - (\mathbf{u}_0 + \varepsilon\Lambda^\varepsilon\Pi_\varepsilon\mathbf{u}_0)\|_{H^1} \le C_3\varepsilon\|\mathbf{F}\|_{L_2}, \quad 0 < \varepsilon \le 1. \end{aligned} \tag{24}$$

Besides $H^1(\mathbb{R}^d;\mathbb{C}^n)$-approximation of the solution $\mathbf{u}_\varepsilon$ (see (24)), it is interesting to find $L_2(\mathbb{R}^d;\mathbb{C}^m)$-approximation for the so called *flux*

$$\mathbf{p}_\varepsilon = g^\varepsilon b(\mathbf{D})\mathbf{u}_\varepsilon. \tag{25}$$

Theorem 7. *Let $\mathbf{u}_\varepsilon$ be the solution of (22), and let $\mathbf{u}_0$ be the solution of (23). Let $\mathbf{p}_\varepsilon$ be defined by (25), and let $\widetilde{g}(\mathbf{x})$ be the matrix (7). Let Π_ε be the operator (17). Then we have*

$$\|\mathbf{p}^\varepsilon - \widetilde{g}^\varepsilon \Pi_\varepsilon b(\mathbf{D})\mathbf{u}_0\|_{L_2} \le C_4 \varepsilon \|\mathbf{F}\|_{L_2}, \quad 0 < \varepsilon \le 1. \tag{26}$$

The constant C_4 in (26) depends only on the norms $\|g\|_{L_\infty}$, $\|g^{-1}\|_{L_\infty}$, on α_0, α_1, and on parameters of the lattice Γ. In (26) the smoothing operator Π_ε can be replaced by I in the same cases as in Theorem 5.

Now, let $\mathbf{w}_\varepsilon$ be the solution of the equation

$$\mathcal{A}_\varepsilon \mathbf{w}_\varepsilon + \mathbf{w}_\varepsilon = \mathbf{F}, \quad \mathbf{F} \in L_2(\mathbb{R}^d; \mathbb{C}^n). \tag{27}$$

Suppose that $\overline{Q}$ is defined in (12), and that $\mathbf{w}_\varepsilon^0$ is the solution of the equation

$$\hat{\mathcal{A}}^0 \mathbf{w}_\varepsilon^0 + \overline{Q}\mathbf{w}_\varepsilon^0 = ((f^\varepsilon)^*)^{-1}\mathbf{F}. \tag{28}$$

The role of the flux for (27) is played by the function

$$\mathbf{r}_\varepsilon = g^\varepsilon b(\mathbf{D}) f^\varepsilon \mathbf{w}_\varepsilon. \tag{29}$$

Theorem 8. *Let $\mathbf{w}_\varepsilon$ be the solution of (27), and let $\mathbf{w}_\varepsilon^0$ be the solution of (28). Let $\mathbf{r}_\varepsilon$ be defined by (29), and let $\widetilde{g}(\mathbf{x})$ be the matrix (7). Suppose that Π_ε is the operator (17). Then we have*

$$\|\mathbf{r}^\varepsilon - \widetilde{g}^\varepsilon \Pi_\varepsilon b(\mathbf{D})\mathbf{w}_\varepsilon^0\|_{L_2} \le C_4^{(Q)} \varepsilon \|\mathbf{F}\|_{L_2}, \quad 0 < \varepsilon \le 1. \tag{30}$$

The constant $C_4^{(Q)}$ depends only on $\|g\|_{L_\infty}$, $\|g^{-1}\|_{L_\infty}$, $\|f\|_{L_\infty}$, $\|f^{-1}\|_{L_\infty}$, α_0, α_1, and on parameters of the lattice Γ. In (30) the smoothing operator Π_ε can be replaced by I in the same cases as in Theorem 5.

Theorems 7 and 8 have been proved in [7].

6 The Method of Investigation

Applying the *Floquet-Bloch theory*, we decompose $\mathcal{A}$ in the direct integral of operators $\mathcal{A}(\mathbf{k})$, acting in $L_2(\Omega; \mathbb{C}^n)$ and depending on the parameter $\mathbf{k} \in \mathbb{R}^d$ called *quasimomentum*. For this we need the *Gelfand transformation* $\mathcal{U}$. First, $\mathcal{U}$ is defined on functions of the Schwartz class by the formula

$$(\mathcal{U}\mathbf{f})(\mathbf{k}, \mathbf{x}) = |\widetilde{\Omega}|^{-1/2} \sum_{\mathbf{a} \in \Gamma} \exp(-i\langle \mathbf{k}, \mathbf{x} + \mathbf{a}\rangle)\mathbf{f}(\mathbf{x} + \mathbf{a}), \quad \mathbf{x} \in \Omega, \ \mathbf{k} \in \widetilde{\Omega},$$

$\mathbf{f} \in \mathcal{S}(\mathbb{R}^d; \mathbb{C}^n)$. Next, $\mathcal{U}$ is extended by continuity to the unitary operator

$$\mathcal{U} : L_2(\mathbb{R}^d; \mathbb{C}^n) \to \int\limits_{\widetilde{\Omega}} \oplus L_2(\Omega; \mathbb{C}^n)\, d\mathbf{k}.$$

The operator $\mathcal{A}(\mathbf{k})$ acting in $L_2(\Omega; \mathbb{C}^n)$ is formally given by the differential expression $\mathcal{A}(\mathbf{x}, \mathbf{D}+\mathbf{k})$ with periodic (in $\mathbf{x}$) boundary conditions. The precise definition of the operator $\mathcal{A}(\mathbf{k})$ is given in terms of the closed quadratic form

$$a(\mathbf{k})[\mathbf{u}, \mathbf{u}] = \int\limits_{\Omega} \langle g(\mathbf{x}) b(\mathbf{D}+\mathbf{k}) f(\mathbf{x})\mathbf{u}, b(\mathbf{D}+\mathbf{k}) f(\mathbf{x})\mathbf{u}\rangle\, d\mathbf{x}, \quad f\mathbf{u} \in \widetilde{H}^1(\Omega; \mathbb{C}^n).$$

(Here the symbol $\langle \cdot, \cdot \rangle$ stands for the standard inner product in $\mathbb{C}^m$.) Using the Fourier series for $f\mathbf{u}$ and conditions (2), (3), it is easy to check that

$$c_0 \int\limits_{\Omega} |(\mathbf{D}+\mathbf{k})(f\mathbf{u})|^2\, d\mathbf{x} \le a(\mathbf{k})[\mathbf{u}, \mathbf{u}] \le c_1 \int\limits_{\Omega} |(\mathbf{D}+\mathbf{k})(f\mathbf{u})|^2\, d\mathbf{x}, \tag{31}$$

for $f\mathbf{u} \in \widetilde{H}^1(\Omega; \mathbb{C}^n)$, where c_0 and c_1 are the same as in (4).

The direct integral decomposition for $\mathcal{A}$ is given by the relation:

$$\mathcal{U}\mathcal{A}\mathcal{U}^{-1} = \int\limits_{\widetilde{\Omega}} \oplus \mathcal{A}(\mathbf{k})\, d\mathbf{k}. \tag{32}$$

Estimates (31) and compactness of the embedding of $\widetilde{H}^1(\Omega; \mathbb{C}^n)$ in $L_2(\Omega; \mathbb{C}^n)$ imply that the resolvent of the operator $\mathcal{A}(\mathbf{k})$ is compact. The spectrum of each operator $\mathcal{A}(\mathbf{k})$ is discrete. By $E_j(\mathbf{k})$, $j \in \mathbb{N}$, we denote consecutive eigenvalues of the operator $\mathcal{A}(\mathbf{k})$, enumerated with multiplicities in non-decreasing order. *The band functions* $E_j(\cdot)$ are continuous and $\widetilde{\Gamma}$-periodic in $\mathbf{k}$. The spectrum of $\mathcal{A}$ has a *band structure*: it consists of closed intervals that are the ranges of the band functions $E_j(\cdot)$. Spectral bands can overlap; at the same time, there may be gaps in the spectrum.

By simple variational arguments, estimates (31) show that the first n bands overlap and have the common bottom: $\min_{\mathbf{k}\in\widetilde{\Omega}} E_j(\mathbf{k}) = E_j(0) = 0$, $j = 1, \dots, n$. At the same time the edge of the $(n+1)$-th band is separated from zero: $\min_{\mathbf{k}} E_{n+1}(\mathbf{k}) > 0$. Moreover, using the lower estimate (31) and variational arguments, we obtain the inequalities

$$E_j(\mathbf{k}) \ge c_* |\mathbf{k}|^2, \quad \mathbf{k} \in \widetilde{\Omega}, \ j = 1, \dots, n, \tag{33}$$

where $c_* = \alpha_0 \|f^{-1}\|_{L_\infty}^{-2} \|h^{-1}\|_{L_\infty}^{-2}$.

We study the family of operators $\mathcal{A}(\mathbf{k})$ in order to approximate the resolvent $(\mathcal{A}(\mathbf{k}) + \varepsilon^2 I)^{-1}$ for small ε. The operators $\mathcal{A}(\mathbf{k})$ depend on the parameter $\mathbf{k} \in \mathbb{R}^d$ analytically. However, if $d > 1$ (parameter $\mathbf{k}$ is multidimensional) and $n > 1$ (the eigenvalue $\lambda = 0$ is multiple eigenvalue of $\mathcal{A}(0)$), then the classical analytic perturbation theory does not work. We suggest the following solution of this difficulty. We view $t = |\mathbf{k}|$ as the main perturbation parameter; herewith, we should make our con-

structions and estimates uniform with respect to the parameter $\boldsymbol{\theta} = t^{-1}\mathbf{k} \in \mathbb{S}^{d-1}$. We study the operator family $\mathcal{A}(\mathbf{k}) = \mathcal{A}(t\boldsymbol{\theta}) = A(t, \boldsymbol{\theta})$ by methods of spectral perturbation theory with respect to the one-dimensional parameter t.

Consider the kernel of the operator $\mathcal{A}(0)$:

$$\mathfrak{N} = \operatorname{Ker} \mathcal{A}(0) = \{\mathbf{u} \in L_2(\Omega; \mathbb{C}^n) : f\mathbf{u} = \mathbf{c} \in \mathbb{C}^n\}, \quad \dim \mathfrak{N} = n.$$

Let P be the orthogonal projection of $L_2(\Omega; \mathbb{C}^n)$ onto the subspace $\mathfrak{N}$.

It is crucial to distinguish the so called *spectral germ* $S(\boldsymbol{\theta})$ of the operator $A(t, \boldsymbol{\theta})$ at $t = 0$. The germ is a selfadjoint operator acting in the finite-dimensional subspace $\mathfrak{N}$. Now we give the *spectral* definition of the germ. By the analytic perturbation theory, for $t \le t^0$ there exist real-analytic (in t) branches of eigenvalues $\lambda_l(t, \boldsymbol{\theta})$ and real-analytic branches of (orthonormal in $L_2(\Omega; \mathbb{C}^n)$) eigenvectors $\varphi_l(t, \boldsymbol{\theta})$ of the operator $A(t, \boldsymbol{\theta})$, $l = 1, \dots, n$:

$$A(t, \boldsymbol{\theta})\varphi_l(t, \boldsymbol{\theta}) = \lambda_l(t, \boldsymbol{\theta})\varphi_l(t, \boldsymbol{\theta}), \quad l = 1, \dots, n, \quad t = |\mathbf{k}| \le t^0.$$

Herewith, the number t^0 is controlled explicitly. Namely, we can take

$$t^0 = (r_0/2)\alpha_0^{1/2}\alpha_1^{-1/2}\|f\|_{L_\infty}^{-1}\|f^{-1}\|_{L_\infty}^{-1}\|h\|_{L_\infty}^{-1}\|h^{-1}\|_{L_\infty}^{-1}, \tag{34}$$

where r_0 is the radius of the ball inscribed in $\widetilde{\Omega}$.

For sufficiently small t_* and $t \le t_*$ we have the convergent expansions:

$$\lambda_l(t, \boldsymbol{\theta}) = \gamma_l(\boldsymbol{\theta})t^2 + \mu_l(\boldsymbol{\theta})t^3 + \cdots, \quad l = 1, \dots, n, \tag{35}$$

$$\varphi_l(t, \boldsymbol{\theta}) = \omega_l(\boldsymbol{\theta}) + t\varphi_l^{(1)}(\boldsymbol{\theta}) + \cdots, \quad l = 1, \dots, n. \tag{36}$$

It follows from (33) that $\gamma_l(\boldsymbol{\theta}) \ge c_* > 0$, $l = 1, \dots, n$. The vectors $\omega_l(\boldsymbol{\theta})$, $l = 1, \dots, n$, form an orthonormal basis in the subspace $\mathfrak{N}$. Numbers $\gamma_l(\boldsymbol{\theta})$ and vectors $\omega_l(\boldsymbol{\theta})$ are the *threshold characteristics* of the operator $A(t, \boldsymbol{\theta})$.

Definition 9. The selfadjoint operator $S(\boldsymbol{\theta}) : \mathfrak{N} \to \mathfrak{N}$ such that

$$S(\boldsymbol{\theta})\omega_l(\boldsymbol{\theta}) = \gamma_l(\boldsymbol{\theta})\omega_l(\boldsymbol{\theta}), \quad l = 1, \dots, n,$$

is called the spectral germ of the operator $A(t, \boldsymbol{\theta})$.

It turns out that the germ is responsible for threshold effects, since it contains information about threshold characteristics of the operator $A(t, \boldsymbol{\theta})$.

It is possible to approximate the resolvent $(A(t, \boldsymbol{\theta}) + \varepsilon^2 I)^{-1}$ for small ε *in the operator norm* in $L_2(\Omega; \mathbb{C}^n)$ in terms of the germ. For $0 < \varepsilon \le 1$ we have

$$\|(A(t, \boldsymbol{\theta}) + \varepsilon^2 I)^{-1} - (t^2 S(\boldsymbol{\theta}) + \varepsilon^2 I_{\mathfrak{N}})^{-1} P\|_{L_2(\Omega) \to L_2(\Omega)} \le \mathcal{C}_1 \varepsilon^{-1}, \quad t \le t^0. \tag{37}$$

This estimate is order-sharp, the constants $\mathcal{C}_1$ and t^0 are controlled explicitly.

It is possible to calculate the germ $S(\boldsymbol{\theta})$. Now we formulate the result for the simpler operator family $\hat{A}(t, \boldsymbol{\theta}) = \hat{\mathcal{A}}(\mathbf{k})$ corresponding to the operator (6). In this case

the germ $\hat{S}(\boldsymbol{\theta})$ can be represented as $\hat{S}(\boldsymbol{\theta}) = b(\boldsymbol{\theta})^* g^0 b(\boldsymbol{\theta})$, $\boldsymbol{\theta} \in \mathbb{S}^{d-1}$, where g^0 is the effective matrix. Next, it turns out that the family $\hat{A}^0(t, \boldsymbol{\theta}) = \hat{\mathcal{A}}^0(\mathbf{k})$ corresponding to the effective operator (8) has the same spectral germ. By (37), this allows to approximate the resolvent $(\hat{\mathcal{A}}(\mathbf{k}) + \varepsilon^2 I)^{-1}$ in terms of the resolvent $(\hat{\mathcal{A}}^0(\mathbf{k}) + \varepsilon^2 I)^{-1}$:

$$\|(\hat{\mathcal{A}}(\mathbf{k}) + \varepsilon^2 I)^{-1} - (\hat{\mathcal{A}}^0(\mathbf{k}) + \varepsilon^2 I)^{-1}\|_{L_2(\Omega) \to L_2(\Omega)} \le \mathcal{C}_2 \varepsilon^{-1}, \quad t \le \hat{t}^0, \quad 0 < \varepsilon \le 1. \tag{38}$$

(It turns out that the value $\hat{t}^0$ for the effective operator may be taken the same as for $\hat{\mathcal{A}}$; $\hat{t}^0$ is given by the formula (34) with $f = \mathbf{1}_n$.)

For $\mathbf{k} \in \widetilde{\Omega}$ and $|\mathbf{k}| = t > \hat{t}^0$ the estimate is trivial: each term in (38) is estimated by constant. Hence, the estimate (38) is true for all $\mathbf{k} \in \widetilde{\Omega}$. Using the Gelfand transformation (see (32)), we conclude that

$$\|(\hat{\mathcal{A}} + \varepsilon^2 I)^{-1} - (\hat{\mathcal{A}}^0 + \varepsilon^2 I)^{-1}\|_{L_2(\mathbb{R}^d) \to L_2(\mathbb{R}^d)} \le C_1 \varepsilon^{-1}, \quad 0 < \varepsilon \le 1. \tag{39}$$

Finally, the result of Theorem 1 follows from (39) by the scale transformation. Let T_ε be the unitary operator in $L_2(\mathbb{R}^d; \mathbb{C}^n)$ given by $(T_\varepsilon \mathbf{f})(\mathbf{x}) = \varepsilon^{d/2} \mathbf{f}(\varepsilon \mathbf{x})$. Then $\hat{\mathcal{A}}_\varepsilon = \varepsilon^{-2} T_\varepsilon^* \hat{\mathcal{A}} T_\varepsilon$, and $(\hat{\mathcal{A}}_\varepsilon + I)^{-1} = \varepsilon^2 T_\varepsilon^* (\hat{\mathcal{A}} + \varepsilon^2 I)^{-1} T_\varepsilon$. Similarly, $(\hat{\mathcal{A}}^0 + I)^{-1} = \varepsilon^2 T_\varepsilon^* (\hat{\mathcal{A}}^0 + \varepsilon^2 I)^{-1} T_\varepsilon$. Thus,

$$\|(\hat{\mathcal{A}}_\varepsilon + I)^{-1} - (\hat{\mathcal{A}}^0 + I)^{-1}\|_{L_2 \to L_2} = \varepsilon^2 \|(\hat{\mathcal{A}} + \varepsilon^2 I)^{-1} - (\hat{\mathcal{A}}^0 + \varepsilon^2 I)^{-1}\|_{L_2 \to L_2}.$$

Combining this with (39), we arrive at (11). This proves Theorem 1.

The study of the resolvent for the operator (10) is based on the identity

$$(\mathcal{A}_\varepsilon + I)^{-1} = (f^\varepsilon)^{-1} (\hat{\mathcal{A}}_\varepsilon + Q^\varepsilon)^{-1} ((f^\varepsilon)^*)^{-1}, \tag{40}$$

where $Q(\mathbf{x}) = (f(\mathbf{x}) f(\mathbf{x})^*)^{-1}$, $Q^\varepsilon(\mathbf{x}) = Q(\varepsilon^{-1}\mathbf{x})$. The generalized resolvent $(\hat{\mathcal{A}}_\varepsilon + Q^\varepsilon)^{-1}$ is studied by the same method as the ordinary resolvent for $\hat{\mathcal{A}}_\varepsilon$. We have the following approximation (obtained in [3]):

$$\|(\hat{\mathcal{A}}_\varepsilon + Q^\varepsilon)^{-1} - (\hat{\mathcal{A}}^0 + \overline{Q})^{-1}\|_{L_2 \to L_2} \le \widetilde{C}_1 \varepsilon, \quad 0 < \varepsilon \le 1.$$

Combining this with (40), we arrive at the result of Theorem 2.

In order to prove Theorem 3, we apply the method described above, but now instead of (37) we have to find more accurate approximation for the resolvent $(A(t, \boldsymbol{\theta}) + \varepsilon^2 I)^{-1}$ in terms of appropriate finite rank operator with the error term of order $O(1)$. This approximation has been found in [5]. Note that, in order to obtain such approximation, we have to take into account terms of order t^3 in the expansions (35) for eigenvalues and terms of order t in the expansions (36) for eigenvectors of the operator $A(t, \boldsymbol{\theta})$. The proof of Theorem 4 is based on more accurate approximation for the generalized resolvent $(\hat{\mathcal{A}}_\varepsilon + Q^\varepsilon)^{-1}$ and on the identity (40).

In order to find $(L_2 \to H^1)$-approximation of the resolvent $(\hat{\mathcal{A}}_\varepsilon + I)^{-1}$, we study the operator $\hat{\mathcal{A}}_\varepsilon^{1/2} (\hat{\mathcal{A}}_\varepsilon + I)^{-1}$ in $L_2(\mathbb{R}^d; \mathbb{C}^n)$ and establish the estimate

$$\|\hat{\mathcal{A}}_\varepsilon^{1/2}\left((\hat{\mathcal{A}}_\varepsilon + I)^{-1} - (\hat{\mathcal{A}}^0 + I)^{-1} - \varepsilon K_1(\varepsilon)\right)\|_{L_2\to L_2} \le C\varepsilon, \quad 0 < \varepsilon \le 1, \quad (41)$$

which implies (20). For the proof of (41), it is possible to apply the scale transformation and develop the method described above. For the proof of estimate (21), we study the operator $\hat{\mathcal{A}}_\varepsilon^{1/2}(\hat{\mathcal{A}}_\varepsilon + Q^\varepsilon)^{-1}$ in $L_2(\mathbb{R}^d;\mathbb{C}^n)$ and use the identity (40). Finally, Theorems 7 and 8 about approximations of the fluxes are deduced from Theorems 5 and 6.

7 Some Applications

The general results are applied to particular periodic operators of mathematical physics. The simplest example is the *acoustics operator*

$$\hat{\mathcal{A}} = \mathbf{D}^* g(\mathbf{x})\mathbf{D} = -\operatorname{div} g(\mathbf{x})\nabla,$$

where $g(\mathbf{x})$ is a periodic positive definite $(d \times d)$-matrix-valued function with real entries. Now $n = 1$, $m = d$, $b(\mathbf{D}) = \mathbf{D}$. The matrix $\Lambda(\mathbf{x})$ is a row: $\Lambda(\mathbf{x}) = i(\Phi_1(\mathbf{x}), \dots, \Phi_d(\mathbf{x}))$, where $\Phi_j(\mathbf{x})$ is a periodic solution of the problem

$$\operatorname{div} g(\mathbf{x})(\nabla\Phi_j(\mathbf{x}) + \mathbf{e}_j) = 0, \qquad \int_\Omega \Phi_j(\mathbf{x})\, d\mathbf{x} = 0.$$

Next, $\widetilde{g}(\mathbf{x})$ is the $(d\times d)$-matrix with the columns $g(\mathbf{x})(\nabla\Phi_j(\mathbf{x})+\mathbf{e}_j)$, $j = 1, \dots, d$, and g^0 is defined as the mean value of the matrix $\widetilde{g}(\mathbf{x})$ over the cell Ω. The effective operator is given by $\hat{\mathcal{A}}^0 = \mathbf{D}^* g^0 \mathbf{D}$. The kernel $\mathfrak{N}$ is one-dimensional and consists of constants: $\mathfrak{N} = \{u \in L_2(\Omega) : u = \text{const}\}$. The spectral germ $S(\boldsymbol{\theta})$ is the operator of multiplication by the number $\gamma(\boldsymbol{\theta}) = \langle g^0\boldsymbol{\theta}, \boldsymbol{\theta}\rangle$. The bottom of the spectrum is realized as the edge of the first band, and the first band function $E_1(\mathbf{k})$ has the following asymptotics: $E_1(\mathbf{k}) = \langle g^0\mathbf{k}, \mathbf{k}\rangle + O(|\mathbf{k}|^4)$, $|\mathbf{k}| \to 0$.

Applying Theorem 1 to the operator $\hat{\mathcal{A}}_\varepsilon = \mathbf{D}^* g^\varepsilon \mathbf{D}$, we obtain

$$\|(\hat{\mathcal{A}}_\varepsilon + I)^{-1} - (\hat{\mathcal{A}}^0 + I)^{-1}\|_{L_2\to L_2} \le C\varepsilon.$$

Theorems 3 and 5 are also applicable. Now the third term of the corrector (15) vanishes. Besides, the corrector does not contain the smoothing operator Π_ε and is given by

$$K(\varepsilon) = K_1(\varepsilon) + K_1(\varepsilon)^*, \quad K_1(\varepsilon) = \sum_{j=1}^d \Phi_j^\varepsilon \partial_j (\hat{\mathcal{A}}^0 + I)^{-1}. \quad (42)$$

Theorems 3 and 5 imply the estimates

$$\|(\hat{\mathcal{A}}_\varepsilon + I)^{-1} - \left((\hat{\mathcal{A}}^0 + I)^{-1} + \varepsilon K(\varepsilon)\right)\|_{L_2 \to L_2} \le C\varepsilon^2,$$
$$\|(\hat{\mathcal{A}}_\varepsilon + I)^{-1} - \left((\hat{\mathcal{A}}^0 + I)^{-1} + \varepsilon K_1(\varepsilon)\right)\|_{L_2 \to H^1} \le C\varepsilon.$$

Finally, Theorem 7 yields the following approximation for the fluxes:

$$\|g^\varepsilon \nabla u_\varepsilon - \widetilde{g}^\varepsilon \nabla u_0\|_{L_2} \le C\varepsilon \|F\|_{L_2}.$$

Here u_ε is the solution of the equation $-\operatorname{div} g^\varepsilon \nabla u_\varepsilon + u_\varepsilon = F$, $F \in L_2(\mathbb{R}^d)$, and u_0 is the solution of the equation $-\operatorname{div} g^0 \nabla u_0 + u_0 = F$.

Now, we consider the *periodic Schrödinger operator* $\mathcal{H}$ with the metric $a(\mathbf{x})$ and potential $p(\mathbf{x})$:

$$\mathcal{H} = \mathbf{D}^* a(\mathbf{x}) \mathbf{D} + p(\mathbf{x}).$$

Here $a(\mathbf{x})$ is $(d \times d)$-matrix-valued function with real entries, $a(\mathbf{x})$ is bounded and positive definite. Potential $p(\mathbf{x})$ is subject to the conditions: $p \in L_s(\Omega)$, where $s = 1$ for $d = 1$ and $2s > d$ for $d \ge 2$. Adding an appropriate constant to the potential $p(\mathbf{x})$, we assume that the bottom of the spectrum of $\mathcal{H}$ is the point $\lambda = 0$. Then there exists a positive periodic solution of the equation $\mathbf{D}^* a(\mathbf{x}) \mathbf{D}\omega + p(\mathbf{x})\omega = 0$. It is convenient to fix the solution ω by the condition $\int_\Omega \omega^2(\mathbf{x})\, d\mathbf{x} = |\Omega|$.

The operator $\mathcal{H}$ admits the following factorization: $\mathcal{H} = \omega^{-1} \mathbf{D}^* a \omega^2 \mathbf{D} \omega^{-1}$. Then $\mathcal{H} = \mathcal{A}(g, f)$ with $g = a\omega^2$ and $f = \omega^{-1}$. Let g^0 be the effective matrix for the acoustics operator $\hat{\mathcal{A}} = \mathbf{D}^* g(\mathbf{x}) \mathbf{D} = \mathbf{D}^* a(\mathbf{x}) \omega^2(\mathbf{x}) \mathbf{D}$, and let $\hat{\mathcal{A}}^0 = \mathbf{D}^* g^0 \mathbf{D}$. Now, the kernel $\mathfrak{N}$ is one-dimensional: $\mathfrak{N} = \{u \in L_2(\Omega) : u = c\omega\}$. The spectral germ $S(\boldsymbol{\theta})$ is the operator of multiplication by the number $\gamma(\boldsymbol{\theta}) = \langle g^0 \boldsymbol{\theta}, \boldsymbol{\theta} \rangle$. For the first band function $E_1(\mathbf{k})$, we have $E_1(\mathbf{k}) = \langle g^0 \mathbf{k}, \mathbf{k} \rangle + O(|\mathbf{k}|^4)$, $|\mathbf{k}| \to 0$. In quantum mechanics the tensor inverse to γ is called the *tensor of effective masses*. Thus, under the conditions $g = a\omega^2$ and $\int_\Omega \omega^2\, d\mathbf{x} = |\Omega|$, the *tensors of effective masses for the Schrödinger operator and for the acoustics operator* $\hat{\mathcal{A}} = \mathbf{D}^* g \mathbf{D}$ *coincide*.

In the one-dimensional case ($d = 1$) with $a(\mathbf{x}) = 1$ (i. e., for the operator $\mathcal{H} = -\frac{d^2}{dx^2} + p(x)$), the number γ is calculated explicitly:

$$\gamma = |\Omega|^2 \|\omega\|^{-2}_{L_2(\Omega)} \|\omega^{-1}\|^{-2}_{L_2(\Omega)}. \tag{43}$$

This formula is well known in quantum mechanics as the formula for the effective mass of the one-dimensional Schrödinger operator at the bottom of the spectrum.

Now, we consider the operator $\mathcal{H}_\varepsilon$ with rapidly oscillating coefficients $\mathcal{H}_\varepsilon = (\omega^\varepsilon)^{-1} \mathbf{D}^* g^\varepsilon \mathbf{D} (\omega^\varepsilon)^{-1}$. In the initial terms, we have $\mathcal{H}_\varepsilon = \mathbf{D}^* a^\varepsilon \mathbf{D} + \varepsilon^{-2} p^\varepsilon$. Theorems 2, 4, 6 and 8 are applicable. Let $\hat{\mathcal{A}}^0 = \mathbf{D}^* g^0 \mathbf{D}$. By the normalization condition on $\omega(\mathbf{x})$, we have $\overline{Q} = 1$. Applying Theorem 2, we obtain

$$\|(\mathcal{H}_\varepsilon + I)^{-1} - \omega^\varepsilon (\hat{\mathcal{A}}^0 + I)^{-1} \omega^\varepsilon\|_{L_2 \to L_2} \le C\varepsilon.$$

Applying Theorems 4 and 6, we obtain the estimates

$$\|(\mathcal{H}_\varepsilon + I)^{-1} - \omega^\varepsilon \left((\hat{\mathcal{A}}^0 + I)^{-1} + \varepsilon K(\varepsilon)\right) \omega^\varepsilon\|_{L_2 \to L_2} \le C\varepsilon^2,$$

$$\|(\omega^\varepsilon)^{-1}(\mathcal{H}_\varepsilon + I)^{-1} - \left((\hat{\mathcal{A}}^0 + I)^{-1} + \varepsilon K_1(\varepsilon)\right) \omega^\varepsilon\|_{L_2 \to H^1} \le C\varepsilon.$$

Here $K(\varepsilon)$ and $K_1(\varepsilon)$ correspond to the operator $\hat{\mathcal{A}} = \mathbf{D}^* g \mathbf{D} = \mathbf{D}^* a \omega^2 \mathbf{D}$ and are defined in (42). The result of Theorem 8 can be also realized for the operator $\mathcal{H}_\varepsilon$; we will not dwell on this.

As it was recently shown by R. G. Shterenberg [11], the magnetic Schrödinger operator with sufficiently small periodic magnetic potential can be also written as $\mathcal{A}(g, f)$ with appropriate (complex-valued) g and f. For this operator we obtain similar results. The difference is that, in general, for the magnetic Schrödinger operator $K_3 \ne 0$ (since coefficients of this operator are complex-valued). See details in [6, Sect. 11] and [7, Sect. 19].

Now we consider the *two-dimensional Pauli operator* $\mathcal{P}$ with the periodic magnetic potential $\mathbf{A}(\mathbf{x}) = \{A_1(\mathbf{x}), A_2(\mathbf{x})\}$. For simplicity, assume that $\mathbf{A} \in C^1$. The operator $\mathcal{P}$ acts in $L_2(\mathbb{R}^2; \mathbb{C}^2)$ and is given by

$$\mathcal{P} = \begin{pmatrix} P_- & 0 \\ 0 & P_+ \end{pmatrix}, \quad P_\pm = (\mathbf{D} - \mathbf{A}(\mathbf{x}))^2 \pm B(\mathbf{x}),$$

where $B(\mathbf{x}) = \partial_1 A_2 - \partial_2 A_1$ is the magnetic field. By the gauge transformation, we subject $\mathbf{A}(\mathbf{x})$ to the conditions $\operatorname{div} \mathbf{A}(\mathbf{x}) = 0$ and $\int_\Omega \mathbf{A}(\mathbf{x})\, d\mathbf{x} = 0$. Then there exists a real-valued Γ-periodic function $\varphi(\mathbf{x})$ such that $\nabla\varphi = \{A_2, -A_1\}$ and $\int_\Omega \varphi(\mathbf{x})\, d\mathbf{x} = 0$. We put

$$f(\mathbf{x}) = \begin{pmatrix} e^{\varphi(\mathbf{x})} & 0 \\ 0 & e^{-\varphi(\mathbf{x})} \end{pmatrix}, \qquad b(\mathbf{D}) = \begin{pmatrix} 0 & D_1 - iD_2 \\ D_1 + iD_2 & 0 \end{pmatrix}.$$

The Pauli operator $\mathcal{P}$ is factorized as $\mathcal{P} = f(\mathbf{x}) b(\mathbf{D}) f^2(\mathbf{x}) b(\mathbf{D}) f(\mathbf{x})$. Thus, the operator $\mathcal{P}$ has the form $\mathcal{A}(g, f)$ with $m = n = 2$, $g = f^2$. The effective matrix is calculated explicitly:

$$g^0 = \underline{g} = \begin{pmatrix} |\Omega| \left(\int_\Omega e^{-2\varphi}\, d\mathbf{x}\right)^{-1} & 0 \\ 0 & |\Omega| \left(\int_\Omega e^{2\varphi}\, d\mathbf{x}\right)^{-1} \end{pmatrix}.$$

The kernel $\mathfrak{N}$ is two-dimensional and is given by

$$\mathfrak{N} = \left\{ u(\mathbf{x}) = \begin{pmatrix} c_1 e^{-\varphi(\mathbf{x})} \\ c_2 e^{\varphi(\mathbf{x})} \end{pmatrix} \right\}.$$

The spectral germ $S(\boldsymbol{\theta})$ *does not depend on* $\boldsymbol{\theta}$ and is operator of multiplication by the number

$$\gamma = |\Omega|^2 \|e^{\varphi}\|^{-2}_{L_2(\Omega)} \|e^{-\varphi}\|^{-2}_{L_2(\Omega)}.$$

This formula is analogous to expression (43) for the effective mass of the one-dimensional Schrödinger operator. First two band functions of the Pauli operator coincide and have the following asymptotics $E_1(\mathbf{k}) = E_2(\mathbf{k}) = \gamma|\mathbf{k}|^2 + O(|\mathbf{k}|^3)$, $|\mathbf{k}| \to 0$. Thus, we observe a hidden symmetry: *the tensor of effective masses for the two-dimensional Pauli operator is scalar*.

Now we consider the operator

$$\mathcal{P}_\varepsilon = f^\varepsilon b(\mathbf{D})(f^\varepsilon)^2 b(\mathbf{D}) f^\varepsilon = \begin{pmatrix} P_{-,\varepsilon} & 0 \\ 0 & P_{+,\varepsilon} \end{pmatrix},$$

where $P_{\pm,\varepsilon} = (\mathbf{D} - \varepsilon^{-1}\mathbf{A}^\varepsilon)^2 \pm \varepsilon^{-2}B^\varepsilon$. Theorem 2 yields approximation for the resolvent $(\mathcal{P}_\varepsilon + I)^{-1}$:

$$\|(\mathcal{P}_\varepsilon + I)^{-1} - \widetilde{f}^\varepsilon(-\gamma\Delta + I)^{-1}\widetilde{f}^\varepsilon\|_{L_2 \to L_2} \le C\varepsilon,$$

where

$$\widetilde{f} = \begin{pmatrix} \widetilde{\omega}_- & 0 \\ 0 & \widetilde{\omega}_+ \end{pmatrix}, \quad \widetilde{\omega}_\pm = c_\pm e^{\pm\varphi}, \quad \|\widetilde{\omega}_\pm\|^2_{L_2(\Omega)} = |\Omega|.$$

Theorems 4, 6 and 8 are also applicable to the operator $\mathcal{P}_\varepsilon$. We will not dwell on detailed formulations here.

Besides examples considered above, the general results are applicable to the *periodic operator of elasticity theory*, which can be written in the form (6) (see [3, Sect. 5.2], [6, Sect. 13], [7, Sect. 21]).

8 On Further Development of the Method

In fact, a significant part of considerations is made on the abstract operator theory level for some class of operators admitting an appropriate factorization. The corresponding abstract material can be found in [3, Chap. 1], [5], [7, Chap. 1]. Next, these abstract results were applied to DO's of the form (5), (6), and specific properties of such DO's were used.

The homogenization problem for the stationary periodic Maxwell system turned out to be the most difficult. In the case where one of coefficients (the dielectric permittivity or the magnetic permeability) is constant, the problem is (partially) reduced to the study of the second order operator $\hat{\mathcal{A}} = \operatorname{rot}\eta(\mathbf{x})^{-1}\operatorname{rot} - \nabla\operatorname{div}$, which admits a factorization of the form (6). Then general results for this class of operators are applicable. This case was studied in [3, Chap. 7], but only in [8] necessary approximations for all physical fields have been found.

The problem is even harder, if both coefficients are non-constant. The corresponding "model" second order operator cannot be written in the form (6) or (5). However, it is possible to apply abstract results from [3, 5, 7]. The homogenization problem for the Maxwell system in the case where both coefficients are variable pe-

riodic matrices was studied in [12, 15, 17]. Finally, in [17] the problem was solved completely; namely, approximations in the $L_2(\mathbb{R}^3;\mathbb{C}^3)$-norm for all physical fields have been found.

The method developed by the authors was also applied to the homogenization of the periodic parabolic Cauchy problem (see [13, 16]).

Besides operators with coefficients periodic in all directions, it is interesting to study homogenization problems in domains like layer, cylinder, etc., when coefficients are periodic only in longitudinal variables. Herewith, the homogenization procedure concerns only longitudinal variables, and coefficients of the effective operator still depend on transversal variables. The model problem of such type was studied in [14]. It turned out that it is possible to apply the method of [3] "layerwise", but additional technical difficulties arise.

The analogue of the homogenization procedure can be associated with an internal gap in the spectrum of the initial operator. The papers [1] and [4] are devoted to these questions.

The papers by the authors stimulated interest to approximation of the resolvent in the homogenization theory with the error estimate in the operator norm. Recently, estimates of the form (11) and (20) were proved by V. V. Zhikov by another (nonspectral) method (see [19–21]).

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ABCD and ODEs

Patrick Dorey, Clare Dunning, Davide Masoero, Junji Suzuki and Roberto Tateo

Abstract We outline a relationship between conformal field theories and spectral problems of ordinary differential equations, and discuss its generalization to models related to classical Lie algebras.

1 Introduction

The ODE/IM correspondence [8, 4, 20, 13] has established a link between two dimensional conformal field theory (CFT) and generalised spectral problems in ordinary differential and pseudo-differential equations. It is based on an equivalence between transfer matrix eigenvalues [1, 2] and Baxter Q-functions in integrable models (IMs), and spectral determinants [19, 22] of ordinary differential equations (ODEs).

In statistical mechanics, the transfer matrix and its largest eigenvalue—denoted by T in the following—are central objects. For example, consider the six-vertex model defined on a square lattice with N columns and N' rows; T can be written in terms of an auxiliary entire function Q through the so-called Baxter TQ relation.

Patrick Dorey
Dept. of Mathematical Sciences, University of Durham, Durham DH1 3LE, UK, e-mail: p.e.dorey@durham.ac.uk

Clare Dunning
IMSAS, University of Kent, Canterbury CT2 7NF, UK, e-mail: t.c.dunning@kent.ac.uk

Davide Masoero
SISSA, via Beirut 2-4, 34014 Trieste, Italy, e-mail: masoero@sissa.it

Junji Suzuki
Department of Physics, Shizuoka University, Ohya 836, SURUGA, Shizuoka, Japan, e-mail: sjsuzuk@ipc.shizuoka.ac.jp

Roberto Tateo
Dip. di Fisica Teorica and INFN, Università di Torino, Via P. Giuria 1, 10125 Torino, Italy, e-mail: tateo@to.infn.it

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Up to an overall constant, Q is completely determined by the knowledge of the positions of its zeros, the Bethe roots, which are constrained by the Bethe ansatz equations (BAE). Subject to some qualitative information on the positions of the Bethe roots, easily deduced by studying systems with small size, the Bethe ansatz leads to a unique set of ground-state roots. In the $N' \to \infty$ limit the free energy per site f is simply related to T by

$$f \sim -\frac{1}{N} \ln T. \tag{1}$$

In [1, 2], Bazhanov, Lukyanov and Zamolodchikov showed how to adapt the same techniques directly to the conformal field theory (CFT) limit of the six-vertex model. In this setting, we consider the conformal field theory with Virasoro central charge $c = 1$ corresponding to the continuum limit of the six-vertex model, defined on an infinitely-long strip with twisted boundary conditions along the finite size direction. The largest transfer matrix eigenvalue T depends on three independent parameters: the (rescaled) spectral parameter ν, the anisotropy η and the twist ϕ. Defining E, M, l, ω, Ω through the following relations

$$\begin{aligned} &E = e^{2\nu}, \qquad \eta = \frac{\pi}{2}\frac{M}{M+1}, \qquad \omega = e^{i\frac{\pi}{M+1}}, \\ &\Omega = \omega^{2M}, \qquad \phi = \frac{(2l+1)\pi}{2M+2} \end{aligned} \tag{2}$$

the resulting TQ relation is

$$T(E,l,M)Q(E,l,M) = \omega^{-\frac{2l+1}{2}} Q(\Omega E,l,M) + \omega^{\frac{2l+1}{2}} Q(\Omega^{-1}E,l,M). \tag{3}$$

The Baxter function Q for this largest eigenvalue is fixed by demanding entirety of both T and Q, and reality, positivity and 'extreme packing' for $l > -1/2$ of the set $\{E_i\}$ of zeros of Q. The BAE follow from the entirety of T and Q via

$$Q(E_i) = 0 \quad \Rightarrow \quad T(E_i)Q(E_i) = 0 \quad \Rightarrow \quad \frac{Q(\Omega E_i)}{Q(\Omega^{-1}E_i)} = -\omega^{2l+1}. \tag{4}$$

Surprisingly, (3) and (4) also emerge from an apparently unrelated context: the study of particular spectral problems for the following differential equation

$$\left(\left(\frac{d}{dx} - \frac{l}{x}\right)\left(\frac{d}{dx} + \frac{l}{x}\right) - x^{2M} + E\right) y(x,E,l) = 0\,, \tag{5}$$

with x and E possibly complex. To see the emergence of (4) from (5), we start from the unique solution $\psi(x,E,l)$ of (5) on the punctured complex plane $x \in \mathbb{C} \setminus \{0\}$ which has the asymptotic

$$\psi \sim x^{-M/2} \exp\left(-\frac{1}{M+1}x^{M+1}\right), \qquad (M > 1) \tag{6}$$

as $|x| \to \infty$ in any closed sector contained in the sector $|\arg x| < \frac{3\pi}{2M+2}$. This solution is entire in E and x. From ψ we introduce a family of solutions to (5) using the 'Sibuya trick' (also known as 'Symanzik rescaling'):

$$\psi_k = \psi(\omega^k x, \Omega^k E, l). \tag{7}$$

In (7), k takes integer values; any pair $\{\psi_k, \psi_{k+1}\}$ constitutes a basis of solutions to (5). An alternative way to characterize a solution to (5) is through its behaviour near the origin $x = 0$. The indicial equation is

$$(\lambda - 1 - l)(\lambda + l) = 0\,, \tag{8}$$

and correspondingly we can define two (generally) independent solutions

$$\chi^+(x, E) = \chi(x, E, l) \sim x^{l+1} + O(x^{l+3})\,, \tag{9}$$

and $\chi^-(x, E) = \chi(x, E, -l-1)$, which transform trivially under Symanzik rescaling as

$$\chi^+_k = \chi^+(\omega^k x, \Omega^k E) = \omega^{(l+1)k}\chi^+(x, E)\,. \tag{10}$$

The trick is now to rewrite $\chi^+_0 = \chi^+(x, E)$ respectively in terms of the basis $\{\psi_0, \psi_1\}$ and $\{\psi_{-1}, \psi_0\}$:

$$2i\chi^+_0 = \omega^{-l-\frac{1}{2}} Q(\Omega E)\psi_0 - Q(E)\omega^{-\frac{1}{2}}\psi_1 \tag{11}$$

$$2i\chi^+_0 = 2i\omega^{l+1}\chi^+_{-1} = \omega^{\frac{1}{2}} Q(E)\psi_{-1} - \omega^{l+\frac{1}{2}} Q(\Omega^{-1}E)\psi_0 \tag{12}$$

where the coefficients has been fixed by consistency among (11), (12) and (10) and

$$Q(E, l) = W[\psi_0, \chi^+_0]. \tag{13}$$

Here $W[f, g] = f\frac{dg}{dx} - g\frac{df}{dx}$ denotes the Wronskian of f and g. Taking the ratio (11)/(12) evaluated at a zero $E = E_i$ of Q leads immediately to the Bethe ansatz equations (4) without the need to introduce the TQ relation, though in this case it can be done very easily (see, for example the recent ODE/IM review article [13]). Correspondingly, χ becomes subdominant at $x \to \infty$ on the positive real axis: $\chi(x, E_i, l) \propto \psi(x, E_i, l)$. The motivation of dealing with χ, instead of ψ (6), is two-fold. Firstly, χ can be obtained by applying the powerful and numerically efficient iterative method proposed by Cheng many years ago [7] in the context of Regge pole theory, and applied to spectral problems of this sort in [11]. To this end we introduce the linear operator L, defined through its formal action

$$L[x^p] = \frac{x^{p+2}}{(p+l)(p-l-1)}. \tag{14}$$

So for any polynomial $\mathscr{P}(x)$ of x,

$$\left(\frac{d}{dx}-\frac{l}{x}\right)\left(\frac{d}{dx}+\frac{l}{x}\right)L[\mathscr{P}(x)]=\mathscr{P}(x), \tag{15}$$

and the basic differential equation (5), with the boundary conditions (9) at the origin, is equivalent to

$$\chi(x,E,l)=x^{l+1}+L\Big[(x^{2M}-E)\chi(x,E,l)\Big]. \tag{16}$$

Equation (16) is solvable by iteration and it allows the predictions of the ODE/IM correspondence to be checked with very high precision.

The initial results of [8, 4, 20] connected conformal field theories associated with the Lie algebra A_1 to (second-order) ordinary differential equations. The generalisation to A_{n-1}-models was established in [21, 9] but it was only recently [12] that the ODE/IM correspondence was generalised to the remaining classical Lie algebras B_n, C_n and D_n. Our attempts to derive generalised TQ relations from the proposed set of pseudo-differential equations were unsuccessful, but a series of well-motivated conjectures led us directly to the BAE, allowing us to establish the relationship between BAE and pseudo-differential equation parameters. Moreover, while the numerics to calculate the analogs of the functions ψ turned out to be very costly in CPU time, the generalisation of Cheng's method proved very efficient and allowed very high precision tests to be performed. This is our second main reason to deal with solutions defined through the behaviour about $x=0$, rather than $x=\infty$.

2 Bethe Ansatz for Classical Lie Algebras

For any classical Lie algebra $\mathfrak{g}$, conformal field theory Bethe ansatz equations depending on a set of $rank(\mathfrak{g})$ twist parameters $\gamma=\{\gamma_a\}$ can be written in a compact form as

$$\prod_{b=1}^{rank(\mathfrak{g})}\Omega^{B_{ab}\gamma_b}\frac{Q^{(b)}_{B_{ab}}(E^{(a)}_i,\gamma)}{Q^{(b)}_{-B_{ab}}(E^{(a)}_i,\gamma)}=-1,\quad i=0,1,2,\dots \tag{17}$$

where $Q^{(a)}_k(E,\gamma)=Q^{(a)}(\Omega^k E,\gamma)$, and the numbers $E^{(a)}_i$ are the (in general complex) zeros of the functions $Q^{(a)}$. In (17) the indices a and b label the simple roots of the Lie algebra $\mathfrak{g}$, and

$$B_{ab}=\frac{(\alpha_a,\alpha_b)}{|\text{long roots}|^2},\quad a,b=1,2,\dots,rank(\mathfrak{g}) \tag{18}$$

where the α's are the simple roots of $\mathfrak{g}$. The constant $\Omega=\exp(i\frac{2\pi}{h^\vee\mu})$ is a pure phase, μ is a positive real number and $h^\vee$ is the dual Coxeter number.

It turns out that the Bethe ansatz roots generally split into multiplets (strings) with approximately equal modulus $|E^{(a)}_i|$. The ground state of the model corresponds to a configuration of roots containing only multiplets with a common dimension $d_a=$

K/B_{aa}; the model-dependent integer K corresponds to the degree of fusion (see for example [16]).

3 The Pseudo-Differential Equations

To describe the pseudo-differential equations corresponding to the A_{n-1}, B_n, C_n and D_n simple Lie algebras we first introduce some notation. We need an nth-order differential operator [9]

$$D_n(\mathbf{g}) = D(g_{n-1} - (n-1))\, D(g_{n-2} - (n-2)) \dots D(g_1 - 1)\, D(g_0), \tag{19}$$

$$D(g) = \left(\frac{d}{dx} - \frac{g}{x}\right), \tag{20}$$

depending on n parameters

$$\mathbf{g} = \{g_{n-1}, \dots, g_1, g_0\}, \qquad \mathbf{g}^\dagger = \{n-1-g_0, n-1-g_1, \dots, n-1-g_{n-1}\}. \tag{21}$$

Also, we introduce an inverse differential operator $(d/dx)^{-1}$, generally defined through its formal action

$$\left(\frac{d}{dx}\right)^{-1} x^s = \frac{x^{s+1}}{s+1}, \tag{22}$$

and we replace the simple 'potential' $P(E, x) = (x^{2M} - E)$ of (5) with

$$P_K(E, x) = (x^{h^\vee M/K} - E)^K. \tag{23}$$

Using the notation of Appendix B in [12] the proposed pseudo-differential equations are reported below.

A_{n-1} models

The A_{n-1} ordinary differential equations are

$$D_n(\mathbf{g}^\dagger)\chi^\dagger_{n-1}(x, E) = P_K(x, E)\chi^\dagger_{n-1}(x, E), \tag{24}$$

with the constraint $\sum_{i=0}^{n-1} g_i = \frac{n(n-1)}{2}$ and the ordering $g_i < g_j < n-1$, $\forall i < j$. We introduce the alternative set of parameters $\gamma = \gamma(\mathbf{g}) = \{\gamma_a(\mathbf{g})\}$

$$\gamma_a = \frac{2K}{h^\vee M}\left(\sum_{i=0}^{a-1} g_i - \frac{a(h^\vee - 1)}{2}\right). \tag{25}$$

The solution $\chi^{\dagger}_{n-1}(x, E)$ is specified by its $x \sim 0$ behaviour

$$\chi^{\dagger}_{n-1} \sim x^{n-1-g_0} + \text{subdominant terms}, \quad (x \to 0^+). \tag{26}$$

In general, this function grows exponentially as x tends to infinity on the positive real axis. In Appendix B of [12], it was shown that the coefficient in front of the leading term, but for an irrelevant overall constant, is precisely the function $Q^{(1)}(E, \gamma)$ appearing in the Bethe Ansatz, that is

$$\chi^{\dagger}_{n-1} \sim Q^{(1)}(E, \gamma(\mathbf{g}))\, x^{(1-n)\frac{M}{2}} e^{\frac{x^{M+1}}{M+1}} + \text{subdominant terms}, \quad (x \to \infty). \tag{27}$$

Therefore, the set of Bethe ansatz roots

$$\{E^{(1)}_i\} \leftrightarrow Q^{(1)}(E^{(1)}_i, \gamma) = 0 \tag{28}$$

coincide with the discrete set of E values in (24) such that

$$\chi^{\dagger}_{n-1} \sim o\big(x^{(1-n)\frac{M}{2}} e^{\frac{x^{M+1}}{M+1}}\big), \quad (x \to \infty). \tag{29}$$

This condition is equivalent to the requirement of absolute integrability of

$$\big(x^{(n-1)\frac{M}{2}} e^{-\frac{x^{M+1}}{M+1}}\big)\chi^{\dagger}_{n-1}(x, E) \tag{30}$$

on the interval $[0, \infty)$. It is important to stress that the boundary problem defined above for the function $\chi^{\dagger}_{n-1}$ (26) is in general different from the one discussed in Sects. 3 and 4 in [12] involving $\psi(x, E)$. The latter function is instead a solution to the adjoint equation of (24) and characterised by recessive behaviour at infinity. Surprisingly, the two problems are spectrally equivalent and lead to identical sets of Bethe ansatz roots.

D_n models

The D_n pseudo-differential equations are

$$\begin{aligned} &D_n(\mathbf{g}^{\dagger})\left(\frac{d}{dx}\right)^{-1} D_n(\mathbf{g})\chi_{2n-1}(x, E) \\ &\quad = \sqrt{P_K(x, E)}\left(\frac{d}{dx}\right)\sqrt{P_K(x, E)}\,\chi_{2n-1}(x, E). \end{aligned} \tag{31}$$

Fixing the ordering $g_i < g_j < h^{\vee}/2$, the $\mathbf{g} \leftrightarrow \gamma$ relationship is

$$\gamma_a = \frac{2K}{h^\vee M}\left(\sum_{i=0}^{a-1} g_i - \frac{a}{2}h^\vee\right), \quad (a = 1, \ldots, n-2) \tag{32}$$

$$\begin{aligned}\gamma_{n-1} &= \frac{K}{h^\vee M}\left(\sum_{i=0}^{n-1} g_i - \frac{n}{2}h^\vee\right),\\ \gamma_n &= \frac{K}{h^\vee M}\left(\sum_{i=0}^{n-2} g_i - g_{n-1} - \frac{n-2}{2}h^\vee\right).\end{aligned} \tag{33}$$

The solution is specified by requiring

$$\chi_{2n-1} \sim x^{h^\vee - g_0} + \text{subdominant terms}, \quad (x \to 0^+), \tag{34}$$

$$\chi_{2n-1} \sim Q^{(1)}(E, \gamma(\mathbf{g}))\, x^{-h^\vee \frac{M}{2}} e^{\frac{x^{M+1}}{M+1}} + \text{subdominant terms}, \quad (x \to \infty). \tag{35}$$

Figure 1 illustrates $\Psi(x, E) = x^{h^\vee \frac{M}{2}} e^{-\frac{x^{M+1}}{M+1}} \chi_{2n-1}(x, E)$ for the first three eigenvalues of the D_4 pseudo-differential equation defined by $K{=}1$, $M = 1/3$ and $\mathbf{g} = (2.95, 2.3, 1.1, 0.2)$.

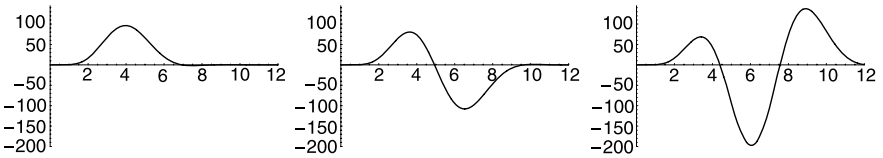

Fig. 1 Lowest three functions $\Psi(x, E)$ for a D_4 pseudo-differential equation

B_n models

The B_n ODEs are

$$D_n(\mathbf{g}^\dagger) D_n(\mathbf{g}) \chi^\dagger_{2n-1}(x, E) = \sqrt{P_K(x, E)}\left(\frac{d}{dx}\right)\sqrt{P_K(x, E)}\,\chi^\dagger_{2n-1}(x, E). \tag{36}$$

With the ordering $g_i < g_j < h^\vee/2$, the $\mathbf{g} \leftrightarrow \gamma$ relation is

$$\gamma_a = \frac{2K}{h^\vee M}\left(\sum_{i=0}^{a-1} g_i - \frac{a}{2}h^\vee\right). \tag{37}$$

The asymptotic behaviours about $x = 0$ and $x = \infty$ are respectively

$$\chi^{\dagger}_{2n-1} \sim x^{h^\vee - g_0} + \text{subdominant terms}, \quad (x \to 0^+)\,, \tag{38}$$

and

$$\chi^{\dagger}_{2n-1} \sim Q^{(1)}(E, \gamma(\mathbf{g}))\, x^{-h^\vee \frac{M}{2}} e^{\frac{x^{M+1}}{M+1}} + \text{subdominant terms}, \quad (x \to \infty). \tag{39}$$

C_n models

The pseudo-differential equations associated to the C_n systems are

$$D_n(\mathbf{g}^\dagger)\left(\frac{d}{dx}\right) D_n(\mathbf{g})\, \chi_{2n+1}(x, E) = P_K(x, E)\left(\frac{d}{dx}\right)^{-1} P_K(x, E)\, \chi_{2n+1}(x, E) \tag{40}$$

with the ordering $g_i < g_j < n$. The relation between the g's and the twist parameters in the BAE is

$$\gamma_a = \frac{2K}{h^\vee M}\left(\sum_{i=0}^{a-1} g_i - an\right), \qquad \gamma_n = \frac{K}{h^\vee M}\left(\sum_{i=0}^{n-1} g_i - n^2\right) \tag{41}$$

and

$$\chi^{\dagger}_{2n+1} \sim x^{2n-g_0} + \text{subdominant terms}, \quad (x \to 0^+), \tag{42}$$

$$\chi^{\dagger}_{2n+1} \sim Q^{(1)}(E, \gamma) x^{-nM} e^{\frac{x^{M+1}}{M+1}} + \text{subdominant terms}, \quad (x \to \infty). \tag{43}$$

Using a generalisation of Cheng's algorithm, the zeros of $Q^{(1)}(E, \gamma)$ can be found numerically and shown to match the appropriate Bethe ansatz roots [12].

In general, the 'spectrum' of a pseudo-differential equation may be either real or complex. In the A_{n-1}, B_n, D_n models with $K = 1$,[1] the special choice $g_i = i$ leads to pseudo-differential equations with real spectra, a property which is expected to hold for a range of the parameters $\mathbf{g}$ (see, for example, [9]). The $K > 1$ generalisation of the potential (23), proposed initially by Lukyanov for the A_1 models [17] but expected to work for all models, introduces a new feature. The eigenvalues corresponding to a $K = 2, 3$ and $K = 4$ case of the $SU(2)$ ODE are illustrated in Fig. 2.

The interesting feature appears if we instead plot the logarithm of the eigenvalues as in Fig. 3. We see that the logarithm of the eigenvalues form 'strings', a well-known feature of integrable models. The string solutions approximately lie along lines in the complex plane, the deviations away from which can be calculated [12] using either WKB techniques, or by studying the asymptotics of the Bethe ansatz equations directly.

[1] The C_n spectrum is complex for any integer $K \geq 1$.

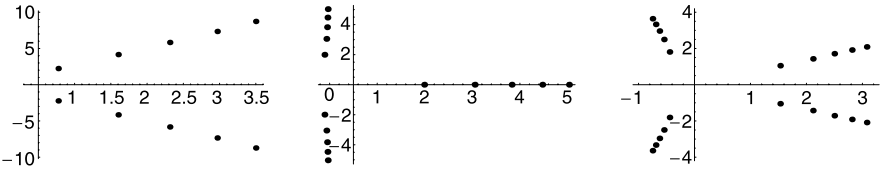

Fig. 2 Complex E-plane: the eigenvalues for the $SU(2)$ model with $M = 3$, $g_0 = 0$ for $K = 2, 3$ and 4 respectively

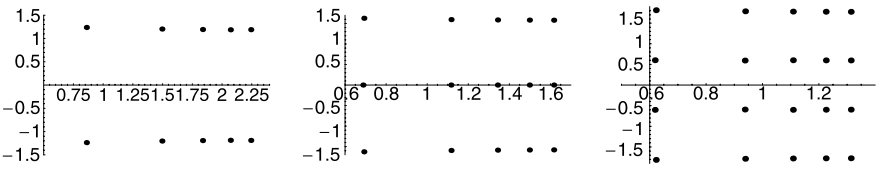

Fig. 3 Complex $(\ln E)$-plane: two, three- and four-strings

To end this section, we would like to comment briefly on the motivation behind the conjectured pseudo-differential equations of B_n, C_n and D_n type. Modulo the generalisation to $K>1$, the A_{n-1} type ODEs were derived in [9]. We began with the D_3 case since it coincides up to relabeling with A_3, implying that the D_3 function $Q^{(1)}(E, \gamma)$ coincides with the A_3 function $Q^{(2)}(E, \gamma)$. Fortunately, the latter is known [9] to encode the spectrum of a differential equation satisfied by the Wronskian of two solutions of the $Q^{(1)}$-related ODE. The generalisation to D_n models with larger n was then clear. Further supporting evidence came from a relationship between certain D_n lattice models and the sine-Gordon model, which appears as an $SU(2)$ problem. This relationship also extends to a set of B_n models, and leads naturally to the full B_n proposal. Finally, the C_n proposal arose from the B_n cases via a consideration of negative-dimension W-algebra dualities [15]. Numerical and analytical tests provided further evidence for the connection between these spectral problems and the Bethe ansatz equations for the classical Lie algebras.

4 Conclusions

The link between integrable models and the theory of ordinary differential equations is an exciting mathematical fact that has the potential to influence the future development of integrable models and conformal field theory, as well as some branches of classical and modern mathematics. Perhaps the most surprising aspect of the functions Q and T, only briefly discussed in this short note, is their variety of possible interpretations: transfer matrix eigenvalues of integrable lattice models in their CFT limit [1, 2], spectral determinants of Hermitian and PT-symmetric [5, 6] spectral problems (see for example [11]), g-functions of CFTs perturbed by relevant boundary operators [1, 10], and particular expectation values in the quantum problem of a

Brownian particle [3]. Further, the (adjoint of the) operators (24), (31), (36) and (40) resemble in form the Miura-transformed Lax operators introduced by Drinfel'd and Sokolov in the context of generalised KdV equations, studied more recently in relation to the geometric Langlands correspondence [18, 14]. Clarifying this connection is an interesting open task. Here we finally observe that the proposed equations respect the well-known Lie algebras relations $D_2 \sim A_1 \oplus A_1$, $A_3 \sim D_3$, $B_1 \sim A_1$, $B_2 \sim C_2$. Also, at special values of the parameters the C_n equations are formally related to the D_n ones by the analytic continuation $n \to -n$, matching an interesting W-algebra duality discussed by Hornfeck in [15]:

$$\frac{(\widehat{D}_{-n})_K \times (\widehat{D}_{-n})_L}{(\widehat{D}_{-n})_{K+L}} \sim \frac{(\widehat{C}_n)_{-K/2} \times (\widehat{C}_n)_{-L/2}}{(\widehat{C}_n)_{-K/2-L/2}}. \tag{44}$$

The relationship between our equations and coset conformal field theories is another aspect worth investigation. We shall return to this point in a forthcoming publication.

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Nonrational Conformal Field Theory

Jörg Teschner

Abstract We introduce a formalism for the construction of correlation functions in certain classes of nonrational conformal field theories. An important role is played by non-degenerate hermitian forms on the spaces of conformal blocks, which allow us to gain some control on the issues coming from the infinite-dimensionality of these spaces. Appropriate generalizations of the concept of a modular functor and of the Friedan-Shenker modular geometry are presented. It is argued that the hermitian form on the spaces of conformal blocks is in fact a scalar product when the representations involved are all unitary, which is illustrated by the case of the $c > 1$ Virasoro conformal blocks.

1 Introduction

In these notes we will discuss the problem to develop a mathematical theory of a certain class of conformal field theories (CFT) which contain the unitary CFT.[1] In similar attempts of this kind the focus mostly was on the so-called *rational* CFT. The author believes that this restriction is unnatural and may obscure where the real issues are. From a physical point of view it seems that *rational* CFT are exceptional rather than generic, owing their existence to some remarkable arithmetic accidents. Although the rational CFT are certainly a mathematically rich and interesting subject in its own right, it seems to the author that the simplifications resulting from rationality obscure what CFTs really are.

The present approach will be based on the so-called gluing construction of the conformal blocks in which one constructs large classes of conformal blocks from the conformal blocks associated to the three punctured sphere. Some aspects of the resulting "Lego-Teichmüller game" are well-understood in the case of rational

Jörg Teschner
DESY Theory, Notkestr. 85, 22603 Hamburg, Germany, e-mail: teschner@mail.desy.de

[1] See [20] to an alternative approach to irrational CFT from a rather different perspective.

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CFT including relations to modular tensor categories, modular functors etc., see [2] and references therein. However, it seems to the author that the gluing construction had not yet been developed for the case of arbitrary Riemann surfaces before. This may be due to the fact that key mathematical results concerning Riemann surface theory like [30] have become available only recently. The author was also unable to find a satisfactory treatment of the consequences of projectiveness of the canonical connection on spaces of conformal blocks within this framework. We will outline an approach to CFT based on the gluing construction that properly deals with these issues.

Of particular importance for us will be to find a proper generalization of the concept of a modular functor which does not assume finite-dimensionality of the spaces of conformal blocks. This immediately raises the issue to control convergence of expansions w.r.t. to a basis for (sub-) spaces of the space of conformal blocks by means of suitable topologies. Also for other reasons it will be seen to be of foundational importance to have a nondegenerate hermitian form, or, in good cases, a scalar product on the spaces of conformal blocks. This is not only required for the construction of correlation functions out of the conformal blocks, it also serves the task to select a subspace of "tempered" conformal blocks among the space of all solutions to the conformal Ward identities. This is one of the main issues which makes the nonrational case much more subtle and interesting than the rational case: As we will illustrate by an example one will generically find that the space of tempered conformal blocks is much smaller than the space of all solutions to the conformal Ward identities. However, the latter contains a subspace of "factorizable" conformal blocks—those that have a reasonable behavior at all boundaries of the moduli space $\mathfrak{M}(\Sigma)$ of complex structures on a given two-dimensional surface Σ. In the example discussed below it turns out that the space of all factorizable conformal blocks can be fully understood[2] provided one understands the much smaller space of all tempered conformal blocks.

The variant of the concept of a modular functor that will be proposed below is based on the consideration of stable surfaces[3] only. This is not usually done in the context of modular functors related to rational CFT, where cutting the surface into pieces containing discs etc. is also allowed. One of the issues that arise is to properly formulate the distinguished role played by insertions of the vacuum representation. This turns out to be somewhat more subtle in nonrational cases.

An important issue is the existence of a canonical nondegenerate hermitian form on spaces of conformal blocks. We will propose a generalization of known relations between the canonical hermitian form and other data characterizing modular functors like the so-called fusion transformation in Sect. 6. Existence of a scalar product on spaces of conformal blocks seems to be an open question even for many rational CFT. In Sect. 6 we will present arguments indicating that the hermitian form gives a scalar product whenever one restricts attention to the conformal blocks associated to *unitary* representations.

[2] Via meromorphic continuation.

[3] Surfaces X with $2g - 2 + n > 0$, with g being the genus of X and n the number of marked points.

It may also be worth mentioning the analogies between CFT and the theory of automorphic forms [39, 14, 15] in which, very roughly speaking, the role of the automorphic forms is taken by the conformal blocks. These analogies play an important role in certain approaches to the geometric Langlands-correspondence, see [15] for a review. An ingredient of the classical theory of automorphic forms that does not seem to have a good counterpart within CFT at the moment is a good analog of the scalar product on spaces of automorphic forms. This structure is the foundation for doing harmonic analysis on spaces of automorphic forms. The author believes that the scalar products on spaces of conformal blocks discussed in this paper provide a natural analog of such a structure.

In any case, one of my aims in this paper will be to advertise the harmonic analysis on spaces of conformal blocks as an attractive future field of mathematical research, naturally generalizing the theory of automorphic forms and the harmonic analysis on real reductive groups.

2 Constraints from Conformal Symmetry

2.1 Motivation: Chiral Factorization of Physical Correlation Functions

A point of view shared by many physicists is that a conformal field theory is characterized by the set of its n-point correlation functions

$$\left\langle V_n(z_n, \bar{z}_n) \dots V_1(z_1, \bar{z}_1) \right\rangle_X , \tag{1}$$

which can be associated to any Riemann surface X with n marked points $z_1, \dots, z_n$ and a collection of vertex operators $V_k(z_k, \bar{z}_k)$ $k = 1, \dots, n$. The vertex operators $V_k(z_k, \bar{z}_k)$ are in one-to-one correspondence with states V_k in representations $\mathfrak{R}_k$ of the conformal symmetry Vir $\times$ Vir by the state-operator correspondence.

A lot of work on CFT was stimulated by the observation that conformal symmetry combined with physical consistency requirements constrain the correlation functions of a CFT strongly.

We will assume that the representations $\mathfrak{R}_k$ factorize as $\mathfrak{R}_k = R_k \otimes R'_k$. It is then sufficient to know the correlation functions in the case that the vectors $V_k \in R_k$ factorize as $V_k = v_k \otimes v'_k \in R_k \otimes R'_k$. The notation $\hat{\Sigma}$ will be used as a short-hand for the topological surface Σ with marked points z_k "decorated" by the representations R_k, R'_k. There are general arguments which indicate that the correlation functions should have a holomorphically factorized structure

$$\left\langle V_n(z_n, \bar{z}_n) \dots V_1(z_1, \bar{z}_1) \right\rangle_X = \int_{\mathbb{F}_{\hat{\Sigma}} \times \mathbb{F}_{\hat{\Sigma}}} d\mu_{\hat{\Sigma}}(S, S') \, \mathscr{F}_S(v; X) \, \overline{\mathscr{F}}_{S'}(v'; X) . \tag{2}$$

This decomposition disentangles the relevant dependencies by encoding them into the following objects:

- The conformal blocks $\mathcal{F}_S(v; X)$ and $\bar{\mathcal{F}}_{S'}(v'; X)$ depend holomorphically and antiholomorphically on the complex structure of the Riemann surface X, respectively. The set $\mathbb{F}_{\hat{\Sigma}}$ of labels S that the integration is extended over will be specified more explicitly below. They furthermore depend on the vectors $v = \bigotimes_{k=1}^n v_k \in \bigotimes_{k=1}^n R_k$ and $v' = \bigotimes_{k=1}^n v'_k \in \bigotimes_{k=1}^n R'_k$, respectively.
- The measure $d\mu_{\hat{\Sigma}}(S, S')$ does not depend on the complex structure of the Riemann surface X but only on its topological type Σ. together with the assignment of representations R_k, R'_k to the punctures z_k.

Given that the correlation functions of a CFT factorize as in (2), it has turned out to be fruitful to approach the construction of correlation function in three steps:

- First construct the conformal blocks $\mathcal{F}_S(v; X)$ by exploiting the constraints coming from the conformal symmetry of the theory.
- Describe the restrictions on the measure $d\mu_{\hat{\Sigma}}(S, S')$ that follow from basic physical consistency requirements (locality, crossing symmetry, modular invariance).
- Identify the solution to these requirements which fulfills further *model-specific* conditions.

We will in the following mainly focus on the first two of these items. Concerning the third let us only remark that the specification of the chiral symmetries will in general not be sufficient to determine the CFT. One may think e.g. of the CFTs with $N = 2$ superconformal symmetry where one expects to find multi-parametric families of such CFTs in general.

2.2 Vertex Algebras

Vertex algebras V represent the chiral symmetries of a CFT. We will require that these symmetries form an extension of the Virasoro algebra

$$[L_n, L_m] = (n-m)L_{n+m} + \frac{c}{12} n(n^2-1)\delta_{n+m,0}\,. \tag{3}$$

A convenient formalism for describing extensions of the conformal symmetry generated by the Virasoro algebra is provided by the formalism of vertex algebras, see [3, 16, 22, 17]. The symmetries are generated from the modes of the "currents" denoted $Y(A, z)$, with formal Laurent-expansion of the form

$$Y(A, z) = \sum_{n\in\mathbb{Z}} A_n z^{-n-1}. \tag{4}$$

There is a canonical Lie algebra $U'(V)$ which can be attached to a vertex algebra V, see [17, Sect. 4.1]. $U'(V)$ is generated from the expansion coefficients A_n introduced in (4).

2.3 Representations of Vertex Algebras

As indicated above, one wants to assign representations of the vertex algebra V to the marked points of Σ. Representations M of the vertex algebra V must in particular be representations of the Lie-algebra $U'(V)$ generated from the coefficients A_n, see [17, Sect. 5] for more details.

Note that V can be considered as a representation of itself, the so-called vacuum representation which is generated from a distinguished vector $v_\circ$ such that $Y(v_\circ, z) = \mathrm{id}$. This realizes the idea of state-operator correspondence: The currents $Y(A, z)$ are in one-to-one correspondence with the states $A \equiv A_{-1}v_\circ$ that they generate from the "vacuum" $v_\circ$ via $\lim_{z\to 0} Y(A, z)v_\circ$. The energy-momentum tensor $T(z) = \sum_{n\in\mathbb{Z}} L_n z^{-n-2}$ is identified with $Y(A, z)$ for $A = L_{-2}v_\circ$.

We will mainly be interested in unitary representations M of the vertex algebra V. To define the notion of a unitary representation of V we need to say how hermitian conjugation should act on the generators of $U'(V)$. Formally this means that we need to assume that V is equipped with a $*$-structure, a conjugate linear anti-automorphism $* : A_n \to A_n^*$ of $U'(V)$ such that $*^2 = \mathrm{id}$. M is a unitary representation of V if it has the structure of a Hilbert space with scalar product $\langle ., . \rangle_M$ such that $A_n^\dagger = A_n^*$. We will assume in particular that $L_n^* = L_{-n}$, as it is usually done to define unitary representations of the Virasoro algebra.

Let $\mathbb{U}$ be the set of all (equivalence classes) of *irreducible* unitary representations with positive energy of V. Following the terminology from Lie group theory we will call $\mathbb{U}$ the unitary dual of V. General unitary representations M can then be parametrized by measures μ_M on $\mathbb{U}$. The corresponding Hilbert space $\mathfrak{H}_M$ consists of all families of vectors $v = (\, v_u \,;\, u \in \mathbb{U}\,)$ such that $v_u \in M_u$ for μ_M-almost all $u \in \mathbb{U}$ which are square-integrable w.r.t.

$$\|v\|^2 = \int_{\mathbb{U}} d\mu_M(u)\ \|v_u\|^2_{M_u}. \tag{5}$$

We will in the following sometimes restrict attention to the example of the Virasoro algebra itself. This may be motivated by the observation that in physics the presence of a large symmetry is a lucky accident rather than generic, but most of our discussion can be generalized to other vertex algebras as well.

2.4 Conformal Blocks

We will start by recalling a definition of the conformal blocks that has become standard in the mathematical literature.

2.4.1 Definition

Let X be a Riemann surface of genus g with n marked points $P_1, \ldots, P_n$ and choices of local coordinates t_k near $P_k, k = 1, \ldots, n$ such that the value $t_k = 0$ parametrizes the point $P_k \in X$.

Definition 1. A Virasoro conformal block is a linear functional $F : M_X \equiv \prod_{r=1}^n M_r \to \mathbb{C}$ that satisfies the following invariance condition:

$$F(T[\eta] \cdot v) = 0, \tag{6}$$

for all $v \in M_X$ and all meromorphic vectors fields η on X that have poles only at $z_1, \ldots, z_n$. The operator $T[\eta]$ is defined as

$$T[\eta] = \sum_{k=1}^{n} \sum_{n \in \mathbb{Z}} \eta_n^{(k)} L_n^{(k)}, \qquad L_n^{(k)} = \mathrm{id} \otimes \ldots \otimes \underset{\text{(k-th)}}{L_n} \otimes \ldots \otimes \mathrm{id}, \tag{7}$$

where the $\eta_n^{(k)}$ are the Laurent expansion coefficients of η near P_k, $\eta(t_k) = \sum_{n \in \mathbb{Z}} \eta_n^{(k)} t_k^{n+1}$.

The definition of conformal blocks for a general conformal vertex algebra V is given in [17]. In addition to the conformal invariance condition formulated in Definition 1 one imposes conditions which express invariance w.r.t. the symmetries generated by the other currents that generate the vertex algebra V.

We then denote by $\mathscr{C}_V(X, R)$ the space of all conformal blocks associated to a vertex algebra V, a Riemann surface X and the assignment R of a representation M_k to each of the marked points z_k on X.

2.4.2 Insertions of the Vacuum Representation

Let us consider the case that one of the marked points $z_0, \ldots, z_n$ is decorated by the vacuum representation V. If e.g. $R_0 = V$ we may compare the space $\mathscr{C}_V(X, R)$ to the space $\mathscr{C}_V(X', R')$ where X' is the Riemann surface obtained from X by "filling" the marked point z_0, and with representations $R_k \in \mathrm{Rep}(V)$, $k = 1, \ldots, n$ assigned to the marked points $z_1, \ldots, z_n$, respectively. It can then be shown that the spaces $\mathscr{F}(X, R)$ and $\mathscr{F}(X', R')$ are canonically isomorphic [17, Theorem 10.3.1]. The isomorphism is defined by demanding that

$$F'(v) = F(v_\circ \otimes v), \tag{8}$$

holds for all $v \in \bigotimes_{k=1}^n R_k$. In other words: Insertions of the vacuum do not change the space of conformal blocks. This innocent looking fact will be referred to as the "propagation of vacua". It has important consequences.

2.4.3 Deformations of the Complex Structure of X

A key point that needs to be understood about spaces of conformal blocks is the dependence on the complex structure of X. There is a canonical way to represent infinitesimal variations of the complex structure on the spaces of conformal blocks. By combining the definition of conformal blocks with the so-called "Virasoro uni-

formization" of the moduli space $\mathfrak{M}_{g,n}$ one may construct a representation of infinitesimal motions on $\mathfrak{M}_{g,n}$ on the space of conformal blocks.

The "Virasoro uniformization" of the moduli space $\mathfrak{M}_{g,n}$ may be formulated as the statement that the tangent space $T\mathfrak{M}_{g,n}$ to $\mathfrak{M}_{g,n}$ at X can be identified with the double quotient

$$T\mathfrak{M}_{g,n} = \Gamma\big(X \setminus \{x_1, \dots, x_n\}, \Theta_X\big) \Big\backslash \bigoplus_{k=1}^{n} \mathbb{C}((t_k))\partial_k \Big/ \bigoplus_{k=1}^{n} \mathbb{C}[[t_k]]\partial_k, \qquad (9)$$

where $\Gamma(X \setminus \{x_1, \dots, x_n\}, \Theta_X)$ is the set of vector fields that are holomorphic on $X \setminus \{x_1, \dots, x_n\}$, while $\mathbb{C}((t_k))$ and $\mathbb{C}[[t_k]]$ are formal Laurent and Taylor series respectively.

Let us then consider $F(T[\eta] \cdot v)$ with $T[\eta]$ being defined in (7) in the case that $\eta \in \bigoplus_{k=1}^{n} \mathbb{C}((t_k))\partial_k$ and $L_r v_k = 0$ for all $r > 0$ and $k = 1, \dots, n$. The defining invariance property (6) together with $L_r v_k = 0$ allow us to define

$$\delta_\vartheta F(v) = F(T[\eta_\vartheta] \cdot v), \qquad (10)$$

where δ_ϑ is the derivative corresponding a tangent vector $\vartheta \in T\mathfrak{M}_{g,n}$ and η_ϑ is any element of $\bigoplus_{k=1}^{n} \mathbb{C}((t_k))\partial_k$ which represents ϑ via (9). Generalizing these observations one is led to the conclusion that derivatives w.r.t. to the moduli parameters of $\mathfrak{M}_{g,n}$ are (projectively) represented on the space of conformal blocks, the central extension coming from the central extension of the Virasoro algebra (3).

It is natural to ask if the infinitesimal motions on $\mathfrak{M}_{g,n}$ defined above can be integrated. The space of conformal blocks would then have the structure of a holomorphic vector bundle with a projectively flat connection[4]. This would in particular imply that locally on $\mathfrak{M}_{g,n}$ one may define families of conformal blocks $X \to F_X$ such that the functions $X \to F_X(v)$ depend holomorphically on the complex structure μ on X.

Examples where this property has been established in full generality are somewhat rare, they include the WZNW-models, the minimal models and certain classes of rational conformal field theories in genus zero. However, from a physicists point of view, a vertex algebra whose conformal blocks do not have this property is pathological. We are not going to assume integrability of the canonical connection in the following.

2.5 Correlation Functions vs. Hermitian Forms

Let us return to our original problem, the problem to construct correlation functions $\langle V_n(z_n, \bar{z}_n) \dots V_1(z_1, \bar{z}_1)\rangle_X$. Assuming a holomorphically factorized structure as in (2), it seems natural to identify $\mathbb{F}_{\hat{\Sigma}}$ with an index set for a "basis"[5] $\{\mathscr{F}_S(v; X);\ S \in$

[4] Projective flatness means flatness up to a central element.

[5] Possibly in the sense of generalized functions.

$\mathbb{F}_{\hat{\Sigma}}\}$ for a subspace $\mathfrak{F}(\hat{\Sigma})$ of the space of solutions to the conformal Ward identities (6) that is defined as follows.

Let us focus attention on the dependence of $\mathscr{F}_S(v; X)$ w.r.t. the label S by using the notation $f_{v,X}(S) \equiv \mathscr{F}_S(v; X)$. The measure $d\mu_{\hat{\Sigma}}$ on $\mathbb{F}_{\hat{\Sigma}} \times \mathbb{F}_{\hat{\Sigma}}$ introduced in (2) allows one to consider the space $\mathfrak{F}(\hat{\Sigma})$ of functions on $\mathbb{F}_{\hat{\Sigma}}$ such that

$$\int_{\mathbb{F}_{\hat{\Sigma}} \times \mathbb{F}_{\hat{\Sigma}}} d\mu_{\hat{\Sigma}}(S, S')(f(S))^* f(S') < \infty. \tag{11}$$

By definition, the space $\mathfrak{F}(\hat{\Sigma})$ comes equipped with a hermitian form $H_{\hat{\Sigma}}$ which allows one to represent the correlation functions in the form

$$\left\langle V_n(z_n, \bar{z}_n) \dots V_1(z_1, \bar{z}_1) \right\rangle_X = H_{\hat{\Sigma}}(f_{v',X}, f_{v,X}). \tag{12}$$

The elements of the space $\mathfrak{F}(\hat{\Sigma})$ are identified with elements of a subspace of the space of conformal blocks by associating to each $f \in \mathfrak{F}(\hat{\Sigma})$ a solution $\mathscr{F}_f$ to the conformal Ward identities via

$$\mathscr{F}_f(v; X) \equiv \int_{\mathbb{F}_{\hat{\Sigma}} \times \mathbb{F}_{\hat{\Sigma}}} d\mu_{\hat{\Sigma}}(S, S')(f(S))^* \mathscr{F}_{S'}(v; X). \tag{13}$$

We are therefore confronted with the task to construct suitable hermitian forms on subspaces of the space of conformal blocks which allow us to represent the correlation functions in the form (12).

3 Behavior Near the Boundary of Moduli Space

It is of particular importance for most applications of CFT within physics to understand the behavior of correlation functions near the boundaries of the moduli space $\mathfrak{M}(\Sigma)$ of complex structures on a given two-dimensional surface Σ. Such boundaries may be represented by surfaces on which a closed geodesic c was shrunk to zero length, thereby pinching a node. Two cases may arise:

(A) Cutting X along c produces two disconnected surfaces X_1 and X_2 with boundary.
(B) Cutting X along c produces a connected surface X' with boundary whose genus is smaller than the genus of X ("pinching a handle").

In the following we will propose certain assumptions which ensure existence of an interpretation of the CFT in question as a quantum field theory with Hilbert space

$$\mathfrak{H}_{\mathrm{CFT}} = \int_{\mathbb{U}^2}^{\oplus} d\mu(r, r') R_r \otimes R_{r'}. \tag{14}$$

These assumptions may be loosely formulated as follows.

In case (A) it is required that there exists a representations of the correlation functions by "inserting complete sets of intermediate states", schematically

$$\left\langle V_n(z_n,\bar{z}_n)\dots V_1(z_1,\bar{z}_1)\right\rangle_X = \sum_{v\in\mathscr{B}} \left\langle 0|\mathsf{O}_{X_1} q^{L_0}\bar{q}^{\bar{L}_0}|v\right\rangle_{X_1}\left\langle v|\mathsf{O}_{X_2}|0\right\rangle_{X_2}, \tag{15}$$

where $\mathsf{O}_{X_r} : \mathfrak{H}_{\mathrm{CFT}} \to \mathfrak{H}_{\mathrm{CFT}}$, $r = 1, 2$ are certain operators associated to the surfaces X_1 and X_2, respectively, and the summation is extended over the vectors v which form a basis $\mathscr{B}$ for the space of states $\mathfrak{H}_{\mathrm{CFT}}$ of the conformal field theory in question.

In case (B) it is required that there exists a representations of the correlation functions as a trace

$$\left\langle V_n(z_n,\bar{z}_n)\dots V_1(z_1,\bar{z}_1)\right\rangle_X = \mathrm{tr}_{\mathfrak{H}_{\mathrm{CFT}}}\left(q^{L_0}\bar{q}^{\bar{L}_0}\mathsf{O}_{X'}\right), \tag{16}$$

where $\mathsf{O}_{X'} : \mathfrak{H}_{\mathrm{CFT}} \to \mathfrak{H}_{\mathrm{CFT}}$ is a certain operator associated to the surface X'.

One may formulate these two conditions more precisely by demanding that the conformal blocks which appear in (2) can be obtained by the gluing construction that we will now describe in more detail.

3.1 Gluing of Riemann Surfaces

For the following it will be more convenient to consider Riemann surfaces whose boundary components are represented by holes with parametrized boundaries rather than marked points with choices of local coordinates around them. Conformal invariance allows to relate the two ways of representing boundary components, see [29] for a mathematical discussion of some of the issues involved.

3.1.1

Let X' be a possibly disconnected Riemann surface with $2m + n$ parametrized boundaries which are labelled as $C_1^+, C_1^-, \dots, C_m^+, C_m^-, B_1, \dots, B_n$. We will assume that the parameterizations of the boundaries $C_r^\pm$, $r = 1, \dots, m$ extend holomorphically to give coordinates $t_r^\pm$ for annular neighborhoods $A_r^\pm$ of $C_r^\pm$ such that the boundaries $C_r^\pm$ are represented by the circles $|t_r^\pm| = 1$, while the coordinates of points in the interior of $A_r^\pm$ satisfy $|t_r^\pm| < 1$. We will furthermore assume that the annuli $A_r^\pm$ are mutually non-intersecting.

We may then define a new Riemann surface X by identifying all the points P_1, P_2 which satisfy

$$t_r^+(P_1)t_r^-(P_2) = q_r, \tag{17}$$

for given complex numbers q_r such that $|q| < 1$ and all $r = 1, \dots, m$. The annuli $A_r^\pm$ are thereby mapped to annuli A_r embedded into the new surface X.

One may apply this construction to a family X'_t of surfaces of the kind above with a set of parameters collectively denoted $t = (t_1, \ldots, t_k)$. This yields a family $X_{q,t}$ of Riemann surfaces that is labelled by the $m+k$ parameters $q = (q_1, \ldots, q_m)$ and t. The family of surfaces obtained in this way contains the nodal surfaces X_d which are obtained when at least one of the q_r equals zero. If X'_t is stable, i.e. if its disconnected components all have a number n of punctures larger than $2-2g$, one gets the nodal surfaces X_d that represent the points of the Deligne-Mumford compactification $\overline{\mathfrak{M}}(\Sigma)$ of the moduli space $\mathfrak{M}(\Sigma)$ of complex structures on surfaces Σ homotopic to X.

3.1.2

It will be important for us to notice that there exists a universal family of this kind: A family X_p of surfaces such that for any other family Y_q of surfaces which contains a nodal surface $Y_{q_\circ}$ isomorphic to X_d there exists a holomorphic map $p = \varphi(q)$, defined in some neighborhood of the point $q_\circ$, such that Y_q and $X_{\varphi(q)}$ are isomorphic (related by a holomorphic map).

More precisely let us consider families $\pi_{\mathscr{U}} : \mathscr{X} \to \mathscr{U}$ of surfaces degenerating into a given nodal surface X_d. This means that π is holomorphic and that $X_p \equiv \pi^{-1}(p)$ is a possibly degenerate Riemann surface for each point p in a neighborhood $\mathscr{U}$ of the boundary component $\partial\overline{\mathfrak{M}}_{g,n}$ containing the nodal surface X_d. Following [30] we will call families $\pi_{\mathscr{U}} : \mathscr{X} \to \mathscr{U}$ as above an unfolding of the degenerate surface X_d. The surface X_d is called the central fiber of the unfolding $\pi_{\mathscr{U}}$.

Let us call a family $\pi_{\mathscr{U}} : \mathscr{X} \to \mathscr{U}$ universal if for any other family $\pi_{\mathscr{V}} : \mathscr{Y} \to \mathscr{V}$ which has a central fiber Y_d isomorphic to X_d, there exists a unique extension of the isomorphism $f : Y_d \to X_d$ to a pair of isomorphisms (holomorphic maps) (φ, ϕ), where $\varphi : \mathscr{V} \to \mathscr{U}$ and $\phi : \mathscr{Y} \to \mathscr{X}$ such that $\pi_{\mathscr{U}} \circ \phi = \varphi \circ \pi_{\mathscr{V}}$.

Theorem 2 — [30] —
A nodal punctured Riemann surface X_d admits a universal unfolding if and only if it is stable, i.e. iff $n > 2-2g$.

It is no loss of generality to assume that the family surfaces X_p are obtained by the gluing construction, so $X_p \equiv X_{q,t}$.

3.1.3

It is possible to apply the gluing construction in the cases where $X' = \bigsqcup_{p=1}^{2g-2+n} S_p$ is the disjoint union of three-holed spheres. One thereby gets families of surfaces X_q parametrized only by the gluing parameters $q = (q_1, \ldots, q_m)$ with m being given as $m = 3g-3+n$. The different possibilities to get surfaces X by gluing three punctured spheres can be parametrized by the choice of a cut system, i.e. a collection $\mathrm{c} = \{c_1, \ldots, c_{3g-3+n}\}$ of nonintersecting simple closed curves on X. X' is reobtained by cutting X along the curves c_r, $r = 1, \ldots, m$. The coordinates

$q = (q_1, \ldots, q_m)$ parametrize a neighborhood $\mathscr{U}_c$ of the point in $\overline{\mathfrak{M}}_{g,n}$ represented by the maximally degenerate surface X_c corresponding to $q = 0$. It is known [23, 21] that one may cover all of $\overline{\mathfrak{M}}_{g,n}$ with the coordinate patches $\mathscr{U}_c$ if one considers all possible cut systems c on X.

One may similarly use the coordinates $\tau = (\tau_1, \ldots, \tau_m)$ such that $q_r = e^{-\tau_r}$ as system of coordinates for subsets of the Teichmüller space $\mathfrak{T}_{g,n}$. One should note, however, that the coordinates τ are not unambiguously determined by the cut system c. Indeed, the coordinates τ' obtained by $\tau'_r = \tau_r + 2\pi i k_r$, $k_r \in \mathbb{Z}$, would equally well do the job.

In order to resolve this ambiguity, one may refine the cut system c by introducing a marking σ of X, a three-valent graph on X such that each curve of the cut system intersects a unique edge of σ exactly once.

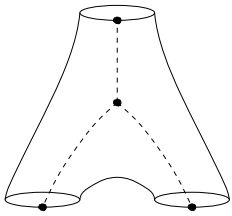

Fig. 1 Standard marking of a three holed sphere

With the help of the graph σ one may then define a "fundamental domain" $\mathscr{V}_\sigma$ for the variables τ as follows: Let us introduce a standard graph like the one depicted in Fig. 1 on each of the three-holed spheres S_p. We may assume that our coordinates are such that the standard graphs in the three holed spheres intersect the boundaries of the annuli A_r in the points $P_r^\pm$ given by $t_r^\pm(P_r^\pm) = |q|$, respectively. On each annulus consider the curve $\gamma_r : [0, 1] \to A_r$, where $t_r^+(\gamma(\theta)) = |q|e^{\tau\theta}$. The curve γ_r connects the points $P_r^\pm$, winding around the annulus A_r a number of times specified by the integer part of $\mathrm{Im}(\tau)/2\pi$. We thereby get a three valent connected graph $\sigma'(\tau)$ on X. The fundamental domain $\mathscr{V}_\sigma$ for the coordinates τ may then be defined by the requirement that the graph $\sigma'(\tau)$ is homotopic to the given graph σ.

3.1.4

It is clear from the definitions that each marking σ determines a cut system $c = c(\sigma)$. The set $\mathscr{M}$ of markings may be regarded as a cover $c : \mathscr{M} \to \mathscr{C}$ of the set $\mathscr{C}$ of all cut systems. The subgroup $\mathrm{MCG}(\Sigma)_c$ of the mapping class group which preserves a cut system c acts transitively on the set of all markings which correspond to the same cut system. The group $\mathrm{MCG}(\Sigma)_c$ is generated by the Dehn twists along the curves c_r, $r = 1, \ldots, 3g - 3 + n$ representing the cut system, together with the braiding transformations of the three holed spheres obtained by cutting X along the

curves c_r, $r = 1, \ldots, 3g - 3 + n$. An example for the braiding transformations is graphically represented in Fig. 2.

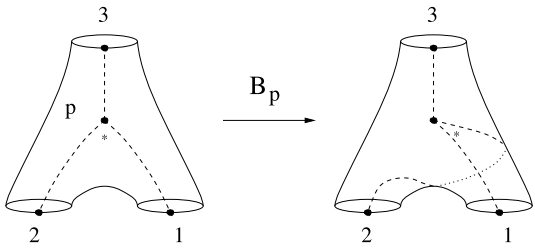

Fig. 2 The B-move

3.2 Gluing of Conformal Blocks

3.2.1

Let us keep the set-up from paragraph 3.1.1. Let R be an assignment of representations of a vertex algebra V to the boundary components of X'_t which is such that representation R_r^- assigned to boundary component C_r^- is the dual of the representation R_r^+ assigned to boundary component C_r^+ for all $r = 1, \ldots, m$. Let $F_t \in \mathscr{C}_V(X'_t; R)$ be a family of conformal blocks assigned to the family X_t of surfaces with an assignment R of representations to the boundary components of X_t as above. Let finally

$$e_\tau \equiv \bigotimes_{r=1}^{m} e_r(\tau_r), \qquad e_r(\tau_r) \equiv \sum_{\imath \in \mathscr{I}_r} e^-_{r,\imath} \otimes e^{-\tau_r L_{0,r}} e^+_{r,\imath},$$

where $\{e^+_{r,\imath}; \imath \in \mathscr{I}_r\}$ and $\{e^-_{r,\imath}; \imath \in \mathscr{I}_r\}$ are bases for R_r^+ and R_r^-, respectively, which are dual to each other in the sense that $\langle e^-_{r,\imath}, e^+_{r,\jmath} \rangle_{R_r^+} = \delta_{\imath,\jmath}$, with $\langle ., . \rangle_{R_r^+}$ being the dual pairing.

We may then consider the expression

$$G_{t,\tau}(v) = F_t(v \otimes e_\tau), \tag{18}$$

where $v_1 \otimes \ldots \otimes v_n$. As it stands, the expression is defined as a formal power series in powers of $e^{-\tau_r}$.

3.2.2

To proceed, we will need to introduce a nontrivial assumption:

The series in (18) have a finite radius of convergence. The resulting domains of definition $\mathscr{D}_\sigma$ of the conformal blocks $G_{t,\tau}$ cover the neighborhoods $\mathscr{U}_{c(\sigma)} \subset \overline{\mathfrak{M}}_{g,n}$ which form an atlas of $\overline{\mathfrak{M}}_{g,n}$ according to [23, 21].

It is not yet clear how large the class of vertex algebras is for which this assumption is satisfied. For rational CFT it is to be expected that the conformal blocks satisfy a closed system of differential equations which allow one to show convergence and existence of an analytic continuation. The situation is more subtle in the case of nonrational CFT. Validity of the assumption above is known [35] in the case of the Virasoro algebra for surfaces with $g = 0$. A key observation is the analyticity of the vector-valued function $e^{-\tau L_0}\psi$ in the cases where the underlying representation of the Virasoro algebra is unitary. Let us also remark that an assumption related to the one above is built into Segal's approach to CFT by requiring that the operators associated to cobordisms are trace-class. For further comments see also Remark 3 at the end of Sect. 3.3 below.

3.2.3 Conformal Ward Identities

We want to check that the expression in (18) satisfies the conformal Ward identities. To this aim it suffices to notice that η can be split as the sum of η_{out} and η_{in}, where η_{out} is holomorphic in X', and η_{in} is holomorphic in $\bigcup_{r=1}^{3g-3+n} A_r$. This means that $G_{t,\tau}(T[\eta]v)$ can be represented as

$$G_{t,\tau}\big(T[\eta]v\big) = F_t\big(T[\eta_{\text{out}}](v \otimes e_\tau)\big) + F_t\big(v \otimes T[\eta_{\text{in}}]e_\tau\big). \tag{19}$$

We have $F_t(T[\eta_{\text{out}}]w) = 0$ for all η_{out} that are holomorphic in X'_t by the conformal Ward identities satisfied by F_t. It is furthermore possible to show that the vectors $e_r(\tau_r)$ are invariant under the action of the holomorphic maps $\eta_{\text{in}}^r \equiv \eta_{\text{in}}|_{A_r}$,

$$T[\eta_{\text{in}}^r]e_r(\tau_r) = 0, \quad r = 1, \ldots, m.$$

The conformal Ward identities follow from the combination of these two observations.

Keeping in mind Theorem 2 it follows from the conformal Ward identities that the conformal blocks defined in (18) do not depend on the choices involved in the gluing construction. The resulting families $G_{t,\tau}$ of conformal blocks are therefore well-defined in a neighborhood $\mathscr{V}_\sigma$ of the component of $\partial\mathfrak{T}_{g,n}$ that is obtained by $\tau_r \to \infty$ for $r = 1, \ldots, m$.

It seems to the author that the foundational importance for CFT of the work [30] was hitherto not as widely appreciated as it should be. It explains in particular why it is absolutely preferable to formulate CFT in terms of stable surfaces.

3.2.4 Decorated Marking Graphs

In the gluing construction above one assigns elements of a basis for the space of conformal blocks of the three punctured sphere to each vertex of a marking graph.

The definition of a basis for this space will generically depend on the choice of a distinguished boundary component of the three punctured sphere in question. In order to parametrize different bases in spaces of conformal blocks one needs to choose for each vertex $p \in \sigma_0$ a distinguished edge emanating from it. The distinguished edge will sometimes be called "outgoing". As a convenient graphical representation we will use the one introduced in Fig. 3. The term marking will henceforth be used for graphs σ as defined above together with the choice of a distinguished edge emanating from each vertex.

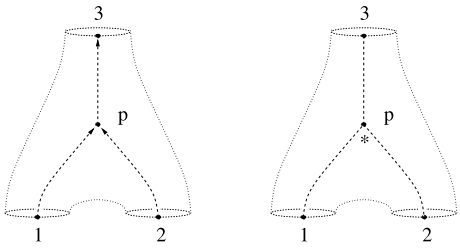

Fig. 3 Two representations for the decoration on a marking graph

3.2.5

The following data label the conformal blocks on X that can be constructed by means of the gluing construction. We will denote by σ_0 and σ_1 the sets of vertices and edges of σ, respectively.

- The marking σ.
- An assignment ρ of representation labels $r_e \in \mathbb{U}$ to the edges $e \in \sigma_1$.
- An assignment w of conformal blocks $w_p \in \mathscr{C}_V(S_p, \rho_p)$ to each vertex $p \in \sigma_0$ of σ with assignment ρ_p of representations to the edges that emanate from p determined by ρ.

We will use the notation $G_{\sigma\tau}(\delta)$ for the family of conformal blocks which is essentially uniquely defined by the data σ and the "decoration" $\delta = (\rho, w)$.

3.3 Correlation Functions

We are now in the position to formulate our requirements concerning the behavior of the correlation functions $\langle V_n(z_n, \bar{z}_n) \dots V_1(z_1, \bar{z}_1)\rangle_X$ near the boundary of moduli space more precisely. Let us consider a marking σ. The marking σ determines a maximally degenerate surface $X_{c(\sigma)}$ and a neighborhood $\mathscr{U}_{c(\sigma)} \subset \overline{\mathfrak{M}}_{g,n}$ of $X_{c(\sigma)}$. Let us recall the set-up from Sect. 2.5, in particular the representation (12). We will adopt the following two requirements:

3.3.1 First Requirement: Factorization of Conformal Blocks

The functions $\mathscr{F}_S(v; X)$ can be identified with the values $G_{\sigma\tau}(\delta|v)$ of the conformal blocks obtained from the gluing construction provided that a suitable identification between the labels S and the decorations δ is adopted. This means in particular that the space $\mathbb{F}_{\hat{\Sigma}}$ of all labels S should be identified with the *sub*-space $\mathscr{I}_{\sigma,R}$ of the space $\mathscr{I}_\sigma$ of all decorations δ which contains all decorations δ_R with fixed assignment R of representations to the external edges[6] of σ.

The space $\mathscr{I}_\sigma$ of all decorations can be described more explicitly as

$$\mathscr{I}_\sigma \equiv \prod_{\rho\in\mathbb{U}^{\sigma_1}} \bigotimes_{p\in\sigma_0} \mathscr{I}_p(\rho_p), \tag{20}$$

where $\mathbb{U}^{\sigma_1}$ is the vector space of all assignments ρ of elements $r_e \in \mathbb{U}$ to the edges $e \in \sigma_1$ and $\mathscr{I}_p(\rho_p)$ is the index set for a basis in $\mathscr{C}(S_p, \rho_p)$, $p \in \sigma_0$.

The role of the functions $f_{v,X}$ from Sect. 2.5 is then taken by the functions $E^R_{\sigma\tau}(v)$ which map a decoration $\delta_R \in \mathscr{I}_{\sigma,R}$ to $G_{\sigma\tau}(\delta_R|v)$. We will later find it more convenient to consider the functions $E_{\sigma\tau}(v) : \mathscr{I}_\sigma \to \mathbb{C}$ which map an *arbitrary* decoration $\delta \in \mathscr{I}_\sigma$ to $G_{\sigma\tau}(\delta|v)$. This is natural in view of the fact that the assignment R of representations to boundary components is part of the data contained in the decoration δ. The space of all complex-valued functions on $\mathscr{I}_\sigma$ will be denoted $\mathfrak{F}_\sigma$.

3.3.2 Second Requirement: Factorization of the Hermitian form $H_{\hat{\Sigma}}$

In order to have a representation for the correlation functions in the form of (12) there must exist a hermitian form $H^{R'R}_\sigma$ on suitable subspaces of $\mathfrak{F}_\sigma \times \mathfrak{F}_\sigma$ such that

$$\big\langle V_n(z_n, \bar{z}_n) \dots V_1(z_1, \bar{z}_1)\big\rangle_X = H^{R'R}_\sigma\big(E_{\sigma\tau}(v'), E_{\sigma\tau}(v)\big). \tag{21}$$

Our second main requirement is that the hermitian form $H^{R'R}_\sigma$ can be factorized as

$$H^{R'R}_\sigma = \int_{\mathbb{U}^{\sigma_1}\times\mathbb{U}^{\sigma_1}} d\mu_{R'R}(\rho', \rho) \bigotimes_{p\in\sigma_0} H_p^{\rho'_p\rho_p}, \tag{22}$$

where

- The measure $d\mu_{R'R}$ has support only when the assignment of representations to the external edges given by ρ' and ρ coincides with R' and R, respectively, and
- The hermitian forms $H_p^{\rho'_p\rho_p}$ are defined on certain subspaces of the spaces $\mathfrak{F}(\rho'_p)\times \mathfrak{F}(\rho_p)$ of complex-valued functions on $\mathscr{I}(\rho'_p) \times \mathscr{I}(\rho_p)$.

Assuming that the hermitian forms $H_p^{\rho'\rho}$ can be represented in the form

[6] The edges ending in the boundary components of Σ.

$$H_p^{\rho'\rho}(f,g) = \sum_{\iota',\iota\in\mathbb{I}} (f(\iota'))^* H_{\iota'\iota}(\rho',\rho) g(\iota), \tag{23}$$

one may in particular represent the three point functions $\langle V_3(y_3,\bar{y}_3)V_2(y_2,\bar{y}_2)V_1(y_1,\bar{y}_1)\rangle_{S_{0,3}}$ as

$$\begin{aligned}&\left\langle V_3(\infty)V_2(1)V_1(0)\right\rangle_{S_{0,3}}\\ &\quad= \sum_{\iota',\iota\in\mathbb{I}} H_{\iota'\iota}(\rho',\rho) G_{\iota'}(\rho'|v_3'\otimes v_2'\otimes v_1') G_\iota(\rho|v_3\otimes v_2\otimes v_1).\end{aligned} \tag{24}$$

In (24) we have used the standard model for $S_{0,3}$ as $\mathbb{P}^1\setminus\{0,1,\infty\}$ and assumed that $y_3=\infty$, $y_2=1$, $y_1=0$. $\{G_{\iota'}(\rho');\iota'\in\mathscr{I}(\rho')\}$ and $\{G_\iota(\rho);\iota\in\mathscr{I}(\rho)\}$ are bases for $\mathscr{C}(S_{0,3}.\rho')$ and $\mathscr{C}(S_{0,3}.\rho)$, respectively.

3.4 Conformal Blocks as Matrix Elements

For future use, let us note that in the case that X has genus zero there is a convenient reformulation of the gluing construction of the conformal blocks in terms of chiral vertex operators.

3.4.1 Chiral Vertex Operators

The chiral vertex operators are families of operators $\Upsilon^{r_2}_{r_3r_1}(\mathfrak{v}_2|z)$, $\mathfrak{v}_2\in R_2$, $z\in\mathbb{C}\setminus\{0\}$ mapping the representation R_{r_1} to the dual $\bar{R}_{r_3}$ of R_{r_3}. They are defined such that the conformal blocks $G^{(3)}$ associated to the three punctured sphere $S^{(3)}$ are related to the matrix elements of $\Upsilon^{r_2}_{r_3r_1}(\mathfrak{v}_2|z)$ as

$$F^{(3)}(\rho|\mathfrak{v}_3\otimes\mathfrak{v}_2\otimes\mathfrak{v}_1) = \left\langle \mathfrak{v}_3, \Upsilon^{r_2}_{r_3r_1}(\mathfrak{v}_2|1)\mathfrak{v}_1\right\rangle_{R_3}. \tag{25}$$

It is assumed that the assignment $\rho: k\mapsto r_k$, $k\in\{1,2,3\}$ is in correspondence to the numbering of boundary components introduced in Fig. 3. A simplified diagrammatical representation is introduced in Fig. 4.

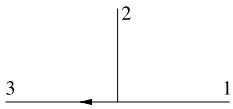

Fig. 4 Diagrammatical representation for chiral vertex operators

The chiral vertex operators $\Upsilon^{r_2}_{r_3r_1}(\mathfrak{v}_2|z)$ are well-defined by (25) in the sense of formal power series in z.

3.4.2

There are two different ways to glue two decorated three-punctured spheres such that the outgoing boundary component of the first is glued to one of the incoming boundary components of the other. To each of the two gluing patterns we may associate two natural ways to compose chiral vertex operators, namely

$$\mathsf{Y}^{r_3}_{r_4 r_{21}}(\mathfrak{v}_3|1)\mathsf{Y}^{r_2}_{r_{21} r_1}(\mathfrak{v}_2|z)\mathfrak{v}_1 \quad \text{and} \quad \mathsf{Y}^{r_{32}}_{r_4 r_1}\big(\mathsf{Y}^{r_3}_{r_3 2 r_2}(\mathfrak{v}_3|1-z)\mathfrak{v}_2|1\big)\mathfrak{v}_1, \tag{26}$$

respectively. A diagrammatic representation for these two ways to compose chiral vertex operators is given in Fig. 5, respectively.

Fig. 5 Diagrammatic representation for the compositions in (26)

Let us call a marking σ on a surface X of genus 0 admissible if the outgoing boundary components of one pair of pants are always glued to an incoming boundary component of another. The resulting markings σ distinguish a unique outgoing boundary component of the surface X. We will assign the representation R_n to this boundary component. Using the rule for compositions of chiral vertex operators recursively we can construct an operator $\mathsf{Y}_{X,\sigma} : R_{n-1} \otimes \cdots \otimes R_1 \to \bar{R}_n$ such that the conformal block associated to σ can be represented as

$$G_\sigma(\mathfrak{v}_n \otimes \cdots \otimes \mathfrak{v}_1) = \big\langle \mathfrak{v}_n, \mathsf{Y}_{X,\sigma}(\mathfrak{v}_{n-1} \otimes \cdots \otimes \mathfrak{v}_1)\big\rangle_{R_n},$$

for all $\mathfrak{v}_k \in R_k$, $k = 1, \ldots, n$. The fact that the matrix elements above represent the conformal blocks follows from the observation that the composition of chiral vertex operators is equivalent to the gluing operation.

Remark 3. The issues of convergence of the power series defined by the gluing construction and convergence of the power series representing the chiral vertex operators are closely related. In rational CFT one can settle this issue with the help of the differential equations satisfied by the conformal blocks, see e.g. [37]. In the case of the Virasoro algebra one may use analytic arguments for deriving such results [35]. The typical situation seems to be that the power series representing, for example, $\langle \mathfrak{v}_{n+1}, \mathsf{Y}^{r_n}_{r_{n+1} s_{n-1}}(\mathfrak{v}_n|z_n) \ldots \mathsf{Y}^{r_1}_{s_1 r_0}(\mathfrak{v}_1|z_1)\mathfrak{v}_0\rangle$ converge provided that the variables z_k are *radially* ordered $|z_n| > \cdots > |z_1|$.

4 From one Boundary to Another

For a given pair of markings σ_2, σ_1 it may happen that the domains $\mathscr{D}_{\sigma_r}$, $r = 1, 2$ in which the corresponding conformal blocks can be defined by means of the gluing

construction have a nontrivial overlap, $\mathscr{D}_{\sigma_2} \cap \mathscr{D}_{\sigma_1} \neq \emptyset$. Assume that τ_1 and τ_2 parametrize the same point in $\mathscr{D}_{\sigma_2} \cap \mathscr{D}_{\sigma_1} \subset \mathfrak{T}_{g,n}$. We then have two possible ways to represent the correlation function $\langle V_n(z_n, \bar{z}_n) \dots V_1(z_1, \bar{z}_1)\rangle_X$ in the form (21), namely either as $H_{\sigma_1}(G_{\sigma_1\tau_1}, G_{\sigma_1\tau_1})$ or as $H_{\sigma_2}(G_{\sigma_2\tau_2}, G_{\sigma_2\tau_2})$, respectively. It is a natural requirement to demand that these two representations agree,

$$H_{\sigma_1}\big(G_{\sigma_1\tau_1}, G_{\sigma_1\tau_1}\big) = H_{\sigma_2}\big(G_{\sigma_2\tau_2}, G_{\sigma_2\tau_2}\big). \tag{27}$$

These constraints generalize what is often called crossing symmetry, locality and modular invariance. Keeping in mind our assumption that the domains $\mathscr{D}_{\sigma_r}$ cover the neighborhoods $\mathscr{U}_{c(\sigma)} \subset \overline{\mathfrak{M}}_{g,n}$ which form an atlas of $\overline{\mathfrak{M}}_{g,n}$ we arrive at an unambiguous definition of the correlation functions on all of $\mathfrak{M}_{g,n}$.

In order to analyze the conditions further, we need to introduce another assumption:

The families $G_{\sigma_1\tau_1}$ and $G_{\sigma_2\tau_2}$ are linearly related.

This assumption will be formulated more precisely below. It is, on the one hand, absolutely necessary for the validity of (27) at least in the case of rational CFT [24][7]. The assumption above is, on the other hand, a rather deep statement about a given vertex algebra V from the mathematical point of view, especially if V is not rational.

What simplifies the analysis somewhat is the fact that the relations between pairs of markings can be reduced to a few simple cases associated to Riemann surfaces of low genus $g = 0, 1$ and low number of marked points $n \leq 4$. In order to explain how this reduction works we will begin by briefly reviewing the necessary results from Riemann surface theory.

4.1 The Modular Groupoid

The physical requirements above boil down to understanding the relations between conformal blocks associated to pairs $[\sigma_2, \sigma_1]$ of markings. In order to break down understanding such relations to a sort of Lego game it will be very useful to observe that all transitions between two markings can be factorized into a simple set of elementary moves. One may formalize the resulting structure by introducing a two-dimensional CW complex $\mathscr{M}(\Sigma)$ with set of vertices $\mathscr{M}_0(\Sigma)$ given by the markings σ, set of edges $\mathscr{M}_1(\Sigma)$ associated to the elementary moves. It will then be possible to identify the set $\mathscr{M}_2(\Sigma)$ of "faces" (relations between the elementary moves) that ensure simply-connectedness of $\mathscr{M}(\Sigma)$, as we are now going to describe in more detail.

[7] It seems likely that the argument in [24] can be generalized to the nonrational case if there exists an analytic continuation of the correlation functions from the euclidean section $\bar{\tau} = \tau^*$ to functions analytic in independent variables $\tau, \bar{\tau}$.

4.1.1 Generators

The set of edges $\mathscr{M}_1(\Sigma)$ of $\mathscr{M}(\Sigma)$ will be given by elementary moves denoted as (pq), Z_p, B_p, F_{pq} and S_p. The indices $p, q \in \sigma_0$ specify the relevant three holed spheres within the pants decomposition of Σ that is determined by σ. The move (pq) will simply be the operation in which the labels p and q get exchanged. Graphical representations for the elementary moves Z_p, B_p, F_{pq} and S_p are given in Figs. 6, 2, 7 and 8, respectively.

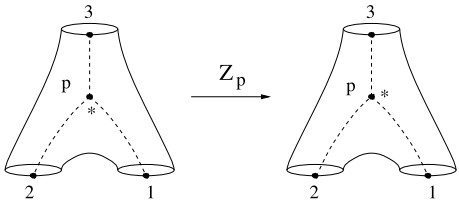

Fig. 6 The Z-move

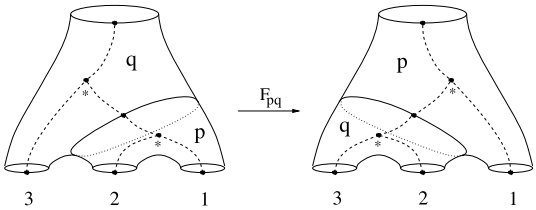

Fig. 7 The F-move

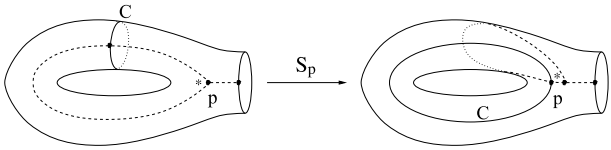

Fig. 8 The S-move

Proposition 4 ([1]). *Any two markings σ, σ' can be connected to each other by a path composed out of the moves (pq), Z_p, B_p, F_{pq} and S_p.*

4.1.2 Relations

It is useful to notice that *any* round trip can be broken up into elementary ones. A complete list of these elementary round trips was first presented in [24], see [1] for a mathematical treatment.

To simplify notation we will write $\pi_2 \sim \pi_1$ if the round trip π in question can be represented as $\pi = \pi_2 \circ \pi_1^{-1}$.

Relations supported on surfaces of genus zero.

$$g = 0,\ s = 3: \quad Z_p \circ Z_p \circ Z_p \sim \mathrm{id}. \tag{28}$$

$$g = 0,\ s = 4: \quad \begin{array}{ll} \text{(a)} & F_{qp} \circ B_p \circ F_{pq} \sim (pq) \circ B_q \circ F_{pq} \circ B_p, \\ \text{(b)} & F_{qp} \circ B_p^{-1} \circ F_{pq} \sim (pq) \circ B_q^{-1} \circ F_{pq} \circ B_p^{-1}, \\ \text{(c)} & A_{pq} \circ A_{qp} \sim (pq). \end{array} \tag{29}$$

$$g = 0,\ s = 5: \quad F_{qr} \circ F_{pr} \circ F_{pq} \sim F_{pq} \circ F_{qr}. \tag{30}$$

We have used the abbreviation

$$A_{pq} \equiv Z_q^{-1} \circ F_{pq} \circ Z_q^{-1} \circ Z_p. \tag{31}$$

Relations supported on surfaces of genus one.

In order to write the relations transparently let us introduce the following composites of the elementary moves.

$$g = 0,\ s = 3: \quad \begin{array}{ll} \text{(a)} & B'_p \equiv Z_p^{-1} \circ B_p \circ Z_p^{-1}, \\ \text{(b)} & T_p \equiv Z_p^{-1} \circ B_p \circ Z_p \circ B_p, \end{array} \tag{32}$$

$$g = 0,\ s = 4: \quad B_{qp} \equiv Z_q^{-1} \circ F_{qp}^{-1} \circ B'_q \circ F_{pq}^{-1} \circ Z_q^{-1} \circ (pq), \tag{33}$$

$$g = 1,\ s = 2: \quad S_{qp} \equiv (F_{qp} \circ Z_q)^{-1} \circ S_p \circ (F_{qp} \circ Z_q). \tag{34}$$

It is useful to observe that the move T_p, represents the Dehn twist around the boundary component of the trinion $\mathfrak{t}_p$ numbered by $i = 1$ in Fig. 3.

With the help of these definitions we may write the relations supported on surfaces of genus one as follows:

$$g = 1,\ s = 1: \quad \begin{array}{ll} \text{(a)} & S_p^2 \sim B'_p, \\ \text{(b)} & S_p \circ T_p \circ S_p \sim T_p^{-1} \circ S_p \circ T_p^{-1}. \end{array} \tag{35}$$

$$g = 1,\ s = 2: \quad B_{qp} \sim S_{qp}^{-1} \circ T_q^{-1} T_p \circ S_{pq}. \tag{36}$$

Theorem 5 – [1] – *The complex $\mathscr{M}(\Sigma)$ is connected and simply connected for any e-surface Σ.*

4.2 Representation of the Generators on Spaces of Conformal Blocks

Definition 6. We will say that a vertex algebra V has the factorization property if

(i) there exists an analytic continuation of the family $G_{\sigma\tau}(\rho, w)$ into a domain in $\mathfrak{T}_{g,n}$ that contains the fundamental domain $\mathscr{V}_\sigma$ in $\mathfrak{T}_{g,n}$.

(ii) For each pair (σ_2, σ_1) of markings related by one of the elementary transformations Z_p, B_P, F_{pq} and S_p there exists a nontrivial intersection $\mathscr{D}_{\sigma_2\sigma_1} \subset \mathfrak{T}_{g,n}$ of the domains $\mathscr{D}_{\sigma_2}$ and $\mathscr{D}_{\sigma_1}$ within which the conformal blocks $G_{\sigma_1\tau_1}(\rho_1, w_1)$ and $G_{\sigma_2\tau_2}(\rho_2, w_2)$ can be uniquely defined by the gluing construction and analytic continuation. There exists a relation of the form

$$G_{\sigma_1\tau_1}(\rho_1, w_1) = \int d\mu_\Sigma(\rho_2) \sum_{w_2} F_{\sigma_1\sigma_2}(\rho_1|\rho_2)^{w_2}_{w_1} G_{\sigma_2\tau_2}(\rho_2, w_2), \tag{37}$$

which holds whenever τ_2, τ_1 parameterize the same point in $\mathscr{D}_{\sigma_2\sigma_1}$.

Let us note that the conjecture can be verified by elementary means in the cases of the moves Z_p and B_p. These are the moves which do not change the cut system. Existence of a relation like (37) for the cases that σ_2 and σ_1 are related by a F_{pq}- or S_p-move is a deep statement. It is, on the one hand, a requirement without which a CFT can hardly be of physical relevance. It may, on the other hand, be hard to prove mathematically that a given vertex operator algebra has this property. Statements of this type are presently only known in the case of certain rational vertex algebras (from the differential equations satisfied by the conformal blocks) or in the nonrational case of the Virasoro algebra reviewed in Sect. 6.

4.2.1

The relation (37) suggests to consider an operator $\mathsf{M}_{\sigma_1\sigma_2}$ between certain subspaces of $\mathfrak{F}_{\sigma_2}$ and $\mathfrak{F}_{\sigma_1}$, respectively, which is defined such that

$$(\mathsf{M}_{\sigma_2\sigma_1} f)_{w_1}(\rho_1) = \int d\mu_\Sigma(\rho_2) \sum_{w_2} F_{\sigma_1\sigma_2}(\rho_1|\rho_2)^{w_2}_{w_1} f_{w_2}(\rho_2). \tag{38}$$

The conditions (27) can be seen to be equivalent to the following condition of invariance of the family of hermitian forms H_σ,

$$H_{\sigma_1}\big(\mathsf{M}_{\sigma_1\sigma_2} f_{\sigma_2}, \mathsf{M}_{\sigma_1\sigma_2} g_{\sigma_2}\big) = H_{\sigma_2}\big(f_{\sigma_2}, g_{\sigma_2}\big). \tag{39}$$

Combined with the factorization (22) one gets nontrivial restrictions on the family of hermitian forms $H^{\rho'\rho}$ on $\mathfrak{F}(\rho') \times \mathfrak{F}(\rho)$.

4.3 Representation of the Relations on Spaces of Conformal Blocks

4.3.1

The operators Z_p, B_p, F_{pq} and S_p defined in the previous subsection are not independent. The faces ϖ of the complex $\mathscr{M}(\Sigma)$ correspond to round trips in $\mathfrak{T}_{g,n}$ starting and ending in the fundamental domain $\mathscr{V}_\sigma$ associated to some marking σ. The realization of such round trip on the conformal blocks can be realized by means of parallel transport w.r.t. the canonical connection on spaces of conformal blocks, in general. The operator $\mathsf{U}(\pi)$ which is associated to a round trip therefore has to be proportional to the identity. It does not have to be equal to the identity since the canonical connection is not flat but only projectively flat. One thereby gets a relation $\mathsf{U}(\varpi) = \xi_\varpi$ between the "generators" Z_p, B_p, F_{pq} and S_p for every round trip ϖ that one can compose out of the elementary moves (pq) Z_p, B_p, F_{pq} or S_p.

4.3.2 Insertions of the Vacuum

Taking into account the propagation of vacua implies that the operators Z_p, B_p, F_{pq} must simplify considerably if one of the representations inserted is the vacuum. We must have, in particular, the relations

$$\mathsf{F} \cdot \left[\mathfrak{H}^0_{\bar{r}_3 r_3} \otimes \mathfrak{H}^{r_3}_{r_2 r_1}\right] = \mathsf{Z} \cdot \mathfrak{H}^{r_1}_{r_3 r_2} \otimes \mathfrak{H}^0_{\bar{r}_1 r_1} \tag{40}$$

$$\mathsf{F} \cdot \left[\mathfrak{H}^{r_3}_{0\bar{r}_3} \otimes \mathfrak{H}^{r_3}_{r_2 r_1}\right] = \mathfrak{H}^{\bar{r}_2}_{0 r_2} \otimes \mathfrak{H}^{r_3}_{r_2 r_1} \tag{41}$$

$$\mathsf{B} \cdot \mathfrak{H}^{\bar{r}}_{0r} = \mathfrak{H}^{\bar{r}}_{r0} \tag{42}$$

$$\mathsf{B} \cdot \mathfrak{H}^0_{r\bar{r}} = \mathsf{T} \cdot \mathfrak{H}^0_{\bar{r}r}. \tag{43}$$

We are using the notation $\mathfrak{H}^{r_3}_{r_2 r_1}$ for $\mathscr{C}(S_{0,3}, \rho)$ if $\rho = (r_3, r_2, r_1)$, with labelling of boundary components in correspondence to the decoration introduced in Fig. 3.

Some of the relations in which these operators appear trivialize accordingly. By rescaling the operators Z_p, B_p, F_{pq} and S_p, if necessary, one can achieve that $\xi_\varpi = 1$ for some other relations. With the help of these observations it is easy to see that one may assume $\xi_\varpi = 1$ for each of the relations (28)–(30) associated to Riemann surfaces of genus zero.

In the case of genus one let us observe that the relation (36) trivializes if one of the two external representations is the vacuum representation. One may furthermore always redefine S_p such that $\xi_\varpi = 1$ in the case of the relation which corresponds to (35), (b). One is left with the relation (35), (a). The arguments well-known from rational CFT [24, 2] lead one to the conclusion that the corresponding relation is

$$\mathsf{S}_p^2 = e^{-\pi i \frac{c}{2}} \mathsf{B}'_p, \tag{44}$$

where c is the central charge of the Virasoro algebra introduced in (3).

5 Notion of a Stable Modular Functor

We shall now formulate an abstract framework that we believe to be suitable for large classes of not necessarily rational CFT. This framework can be seen as a variant of the concept of a modular functor from [33]. Combined with the gluing construction of the conformal blocks it will be shown to yield a concrete realization of the point of view of Friedan and Shenker [18] who proposed to view the partition function of a CFT as a hermitian metric on a projective line bundle over the moduli space of Riemann surfaces, with expectation value of the stress-energy tensor being the canonical connection.

An important feature is that we will assume existence of a scalar product on the spaces of conformal blocks. The topology defined by the scalar product gives us control on the possible infinite-dimensionality of these spaces. Existence of a scalar product may seem to be an overly strong assumption, but we will discuss in the following sections why we believe that the class of vertex algebras that is covered by our formalism is rather large.

5.1 Towers of Representations of the Modular Groupoid

Definition 7. A tower of representations of the modular groupoid assigns to a topological surface Σ the following objects:

- The family of Hilbert spaces $[\mathfrak{H}_\sigma]_{\sigma \in \mathscr{M}_0(\Sigma)}$ of the form

$$\mathfrak{H}_\sigma \equiv \int_{\mathbb{U}^{\sigma_1}}^{\oplus} d\mu_\sigma(\rho) \bigotimes_{p \in \sigma_0} \mathfrak{F}(\rho_p), \tag{45}$$

  where $d\mu_\sigma(\rho)$ is the product measure $d\mu_\sigma(\rho) = \prod_{e \in \sigma_1} d\mu_{\mathrm{Pl}}(r_e)$ if $\rho : \sigma_1 \ni e \to r_e \in \mathbb{U}$.
- For each pair $[\sigma_2, \sigma_1]$ of markings a unitary operator $\mathsf{M}_{\sigma_2\sigma_1} : \mathfrak{H}_{\sigma_1} \to \mathfrak{H}_{\sigma_2}$ such that

$$\mathsf{M}_{\sigma_1\sigma_3} \cdot \mathsf{M}_{\sigma_3\sigma_2} \cdot \mathsf{M}_{\sigma_2\sigma_1} = \xi_{\sigma_3\sigma_2\sigma_1} \cdot \mathrm{id}, \qquad \mathsf{M}_{\sigma_1\sigma_2} \cdot \mathsf{M}_{\sigma_2\sigma_1} = 1, \tag{46}$$

  where $\xi_{\sigma_3\sigma_2\sigma_1} \in \mathbb{C}$, $|\xi_{\sigma_3\sigma_2\sigma_1}| = 1$.

This assignment is such that the following requirements hold:

Disjoint union: Let $X = X' \sqcup X''$ be the disjoint union of X' and X'', and let $\sigma_i = \sigma'_i \sqcup \sigma''_i$, $i = 1, 2$ be two markings on X. Then

$$\mathfrak{H}_\sigma = \mathfrak{H}_{\sigma'} \otimes \mathfrak{H}_{\sigma''}, \tag{47}$$

$$\mathsf{M}_{\sigma_2\sigma_1} = \mathsf{M}_{\sigma_2'\sigma_1'} \otimes \mathsf{M}_{\sigma_2''\sigma_1''}. \tag{48}$$

Gluing: Assume that X' is obtained from X by gluing the boundary components B_2 and B_1. Let σ be a marking on X with edges e_2 and e_1 ending in B_2 and B_1, respectively, and let σ' be the marking on X obtained from σ by gluing e_2 and e_1.

There is a dense subset $\mathscr{T}_\sigma$ of $\mathfrak{H}_\sigma$ such that for each $\Psi \in \mathscr{T}_\sigma$ the following gluing projection is well defined:

$$\mathsf{G}_{e_2e_1}\Psi = \Psi|_{r_{e_2}=r_{e_1}},$$

where $\Psi|_{r_{e_2}=r_{e_1}}$ is obtained from Ψ by restricting it to the subset of $\mathscr{I}_\sigma$ where $r_{e_1} = r_{e_2}$.

The projection $\mathsf{G}_{e_2e_1}$ is then required to be compatible with the representations of the modular groupoids of X and X' in the following sense: It is required that $\mathsf{M}_{\sigma_2\sigma_1}$ maps from $\mathscr{T}_{\sigma_1}$ to $\mathscr{T}_{\sigma_2}$ and that

$$\mathsf{G}_{e_2e_1}\mathsf{M}_{\sigma_2\sigma_1}\Psi = \mathsf{M}_{\sigma_2'\sigma_1'}\mathsf{G}_{e_2e_1}\Psi, \tag{49}$$

holds for all pairs (σ_2', σ_1') of markings on X obtained from the corresponding markings (σ_2, σ_1) on X by gluing, and all $\Psi \in \mathscr{T}_{\sigma_1}$.

Propagation of vacua: Let X' be obtained from X by gluing a disc into the boundary component B_o. Let σ be a marking of X, e_o be the edge of σ that ends in B_o and p_o be the vertex from which e_o emanates. One gets a marking σ' on X' by deleting e_o and p_o and gluing the other two edges that emanate from p_o into a single edge of σ'.

There then exist dense subsets $\mathscr{T}_\sigma$ and $\mathscr{T}_{\sigma'}$ of $\mathfrak{H}_\sigma$ and $\mathfrak{H}_{\sigma'}$, respectively, together with projection mappings $P_{\sigma,B_o} : \mathscr{T}_\sigma \mapsto \mathscr{T}_{\sigma'}$ such that

$$\mathsf{P}_{\sigma_2,B_o}\mathsf{M}_{\sigma_2\sigma_1}\Psi = \mathsf{M}_{\sigma_2'\sigma_1'}\mathsf{P}_{\sigma_1,B_o}\Psi, \tag{50}$$

holds for all pairs (σ_2, σ_1) of markings on X and the corresponding markings (σ_2', σ_1') on X' defined above.

The requirements concerning disjoint union and gluing imply that the representations of the modular groupoids are constructed out of the representatives of the elementary moves B_p, Z_p, F_{pq} and S_p. A tower of representations of the modular groupoid is therefore characterized by the following data:

- The measure set $\mathbb{U}$ (labels of unitary representations of V), equipped with a measure $d\mu_{\mathrm{Pl}}$.
- The Hilbert spaces $\mathfrak{H}_\sigma^{(3)}(\rho)$ associated to the markings σ on the three punctured sphere $\Sigma_{0,3}$ with assignment $\rho : k \mapsto r_k$, $k \in \{1, 2, 3\}$.
- The operators Z, B, F and S mapping $\mathfrak{H}_{\sigma_1}(\rho)$ to $\mathfrak{H}_{\sigma_2}(\rho)$ with respective markings σ_1 and σ_2 being chosen as depicted in Figs. 6–8.

Let us furthermore remark that the constraints imposed on these data by the propagation of vacua requirement are related to (40)–(43). The precise relationship can be subtle if the vacuum representation is not contained in support of $d\mu_{\mathrm{PL}}$ as it may happen for nonrational CFT (see Sect. 6 for an example). The definition of the projection mappings $P_{\sigma,B_\circ}$ then involves analytic continuation w.r.t. the conformal dimensions of the representations, and the compatibility condition (50) requires that the dependence of Z, B, F and S on the labels of external representations has a sufficiently large domain to analyticity.

5.2 Unitary Modular Functors

Given a tower of representations of the modular groupoids there is a canonical way to construct a corresponding modular functor, as we shall now explain. The main issue is to eliminate the apparent dependence on the choice of the marking σ.

Each of the spaces $\mathfrak{H}_\sigma$ becomes a representation of the mapping class group $\mathrm{MCG}(\Sigma)$ by choosing for each $m \in \mathrm{MCG}(\Sigma)$ a sequence π_m of elementary moves that connects σ to $m(\sigma)$. Taking advantage of the fact that the isomorphism $\mathfrak{H}_\sigma \simeq \mathfrak{H}_{m(\sigma)}$ is canonical one gets an operator $\mathsf{M}(m)$ on $\mathfrak{H}_\sigma$.

It is easily seen that for each pair $[\sigma_2, \sigma_1]$ there exist numbers $\zeta_{\sigma_2\sigma_1}$ which satisfy

$$\zeta_{\sigma_1\sigma_3} \cdot \zeta_{\sigma_3\sigma_2} \cdot \zeta_{\sigma_2\sigma_1} = \xi_{\sigma_3\sigma_2\sigma_1} \cdot \mathrm{id}. \tag{51}$$

Indeed, given a fixed reference marking $\sigma_\circ$ one may take e.g. $\zeta_{\sigma_2\sigma_1} \equiv \xi^{-1}_{\sigma_2\sigma_\circ\sigma_1}$. This means that one can use the numbers $\zeta_{\sigma_2\sigma_1}$ to define a *projective* holomorphic line bundle $\mathscr{L}_V$ over $\mathfrak{T}_{g,n}$. To this aim, use the $\mathscr{V}_\sigma$ as local coordinate patches, with transition functions $\zeta_{\sigma_2\sigma_1}$. Projectiveness follows from the nontriviality of the phase $\xi_{\sigma_3\sigma_2\sigma_1}$ associated to triples of markings.

Definition 8. Let $\mathfrak{H}(\Sigma)$ be the Hilbert space whose elements Φ are collections of vectors $\Psi_\sigma \in \mathfrak{H}_\sigma$ such that

$$\Psi_{\sigma_2} = \zeta^{-1}_{\sigma_2\sigma_1} \mathsf{M}_{\sigma_2\sigma_1} \Psi_{\sigma_1}, \tag{52}$$

holds for all pairs of markings σ_1, σ_2 and a given collection of complex numbers $\zeta_{\sigma_2\sigma_1}$ of modulus one which satisfy (51).

For a given collection of numbers $\eta_\sigma \in \mathbb{C}$, $\sigma \in \mathscr{M}_\circ(\Sigma)$, $|\eta_\sigma| = 1$, let us call the operation $\Psi_\sigma \to \eta_\sigma \Psi_\sigma$ for all $\Psi_\sigma \in \mathfrak{H}_\sigma$ a gauge transformation. We will identify the Hilbert spaces $\mathfrak{H}(\Sigma)$ related by gauge transformations.

Let $\rho(\Sigma)$ be the family of mapping class group representations $(\rho_\sigma(R))_{\sigma\in\mathscr{M}_\circ(\Sigma)}$ on the spaces $\mathfrak{H}_\sigma(R)$ modulo the equivalence relation $\sim$ that is induced by the identifications (52).

The assignment $\Sigma \to (\mathfrak{H}(\Sigma), \mathsf{M}(\Sigma))$ will be called a stable unitary projective functor.

5.3 Similarity of Modular Functors

For rational CFT there exist deep results on the equivalence of modular functors from conformal field theory to similar objects coming from quantum group theory [9]. In order to formulate analogous statements about nonrational CFT we will propose the following natural notion of similarity of modular functors.

Definition 9. We will call two modular functors $\mathscr{F}$ and $\mathscr{F}'$ with data

$$\begin{bmatrix}\mathbb{U}\,, d\mu_{\rm Pl}, \mathfrak{H}^{(3)}_\sigma(\rho), \mathsf{Z}\,, \mathsf{B}\,, \mathsf{F}\,, \mathsf{S}\,\end{bmatrix}$$
$$\begin{bmatrix}\mathbb{U}', d\nu_{\rm Pl}, \mathfrak{K}^{(3)}_\sigma(\rho'), \mathsf{Z}', \mathsf{B}', \mathsf{F}', \mathsf{S}'\end{bmatrix}$$

similar iff the following conditions are satisfied:

- There exists a bijection between $\mathbb{U}$ and $\mathbb{U}'$. The measures $d\mu_{\rm Pl}$ and $d\nu_{\rm Pl}$ are equivalent, i.e. there exists a positive function $m(r)$ on $\mathbb{U}$ such that

$$d\mu_{\rm Pl}(r) = m(r) d\nu_{\rm Pl}.$$

- There exist families of invertible operators $\mathsf{E}^{0,3}(\rho) : \mathfrak{H}^{(3)}(\rho) \to \mathfrak{K}^{(3)}(\rho')$, the dependence on each representation label $r_k \in \mathbb{U}$, $k = 1, 2, 3$ measurable w.r.t. $d\mu_{\rm Pl}(s)$ such that the operators $\mathsf{E}_\sigma : \mathfrak{H}_\sigma \to \mathfrak{K}_\sigma$ defined as

$$\mathsf{E}_\sigma \equiv \int_{\mathbb{U}^{\sigma_1}}^{\oplus} d\nu_\sigma(\rho) \prod_{p\in\sigma_0} \mathsf{E}^{0,3}(\rho_p) \tag{53}$$

  are invertible.
- The resulting operators $\mathsf{E}_\sigma : \mathfrak{H}_\sigma \to \mathfrak{K}_\sigma$ satisfy

$$\mathsf{M}'_{\sigma_2\sigma_1} = \mathsf{E}_{\sigma_2} \cdot \mathsf{M}_{\sigma_2\sigma_1} \cdot \mathsf{E}^{-1}_{\sigma_1}.$$

5.4 Friedan-Shenker Modular Geometry

Let us temporarily restrict attention to surfaces X with one marked point at position $z \in X$, decorated with the vacuum representation V. We will assume that the values of the conformal blocks $G_{\sigma\tau}(\delta|v)$ at a given vector $v \in V$ may be considered as a family $(G_{\sigma\tau}(v))_{\tau\in\mathscr{V}_\sigma}$ of elements of the Hilbert space $\mathfrak{H}_\sigma$.

Out of $(G_{\sigma\tau}(v))_{\tau\in\mathscr{V}_\sigma}$ one may then define a collection of vectors $\{\Psi_{\sigma;\sigma'}(v|\tau);$ $\sigma' \in \mathscr{M}_0(\Sigma)\}$, where $\Psi_{\sigma;\sigma'}(v|\tau) \in \mathfrak{H}_{\sigma'}$ for all $\sigma' \in \mathscr{M}_0(\Sigma)$ such that the conditions

$$\Psi_{\sigma;\sigma_2}(v|\tau) = \zeta^{-1}_{\sigma_2\sigma_1} \mathsf{M}_{\sigma_2\sigma_1} \Psi_{\sigma;\sigma_1}(v|\tau) \quad \text{and} \quad \Psi_{\sigma;\sigma}(v|\tau) = G_{\sigma\tau}(v) \in \mathfrak{H}_\sigma \tag{54}$$

are satisfied. Indeed, consistency of the definition of $\Psi_{\sigma;\sigma'}(v|\tau)$ implied by (54) follows from (46) and (51). Let $(\Psi_{\sigma\tau}(v))_{\tau\in\mathscr{V}_\sigma}$ be the holomorphic family of vectors

in $\mathfrak{H}(\Sigma)$ which is associated by Definition 8 to the collection $\{\Psi_{\sigma;\sigma'}(v|\tau);\, \sigma' \in \mathscr{M}_0(\Sigma)\}$.

Given two markings σ_2, σ_1 such that $\mathscr{V}_{\sigma_2} \cap \mathscr{V}_{\sigma_1} \neq \emptyset$ it is easy to see that the families of vectors $(\Psi_{\sigma_2\tau_2}(v))_{\tau_2\in\mathscr{V}_{\sigma_2}}$ and $(\Psi_{\sigma_1\tau_1}(v))_{\tau_1\in\mathscr{V}_{\sigma_1}}$ are related as

$$\Psi_{\sigma_2\tau}(v) = \zeta_{\sigma_2\sigma_1}\Psi_{\sigma_1\tau}(v) \tag{55}$$

if τ_2 and τ_1 parametrize the same point in $\mathscr{V}_{\sigma_2} \cap \mathscr{V}_{\sigma_1}$. Indeed, we had defined $\mathsf{M}_{\sigma_2\sigma_1}$ in (37), (38) such that $G_{\sigma_1\tau_1}(v)=\mathsf{M}_{\sigma_1\sigma_2}G_{\sigma_2\tau_2}(v)$. This implies

$$\begin{aligned}\Psi_{\sigma_1;\sigma_1}(v|\tau_1) \;&=\; G_{\sigma_1\tau_1}(v) = \mathsf{M}_{\sigma_1\sigma_2}G_{\sigma_2\tau_2}(v) = \mathsf{M}_{\sigma_1\sigma_2}\Psi_{\sigma_2;\sigma_2}(v|\tau_2)\\ &\overset{(52)}{=} \zeta_{\sigma_1\sigma_2}\Psi_{\sigma_2;\sigma_1}(v|\tau_2).\end{aligned}$$

This means that for each σ one may regard the family $(\Psi_{\sigma\tau}(v))_{\tau\in\mathscr{V}_\sigma}$ as a local holomorphic section of the projective line bundle $\mathscr{L}_V$ over $\mathfrak{T}_{g,n}$.

The invariance conditions (39) imply that the family of hermitian forms H_σ defines a hermitian form H on $\mathfrak{H}(\Sigma)$. Objects of particular interest for the case at hand are the partition function $Z_g(X)$,

$$Z_g(X) \equiv H\big(\Psi_{\sigma\tau}(v_\circ), \Psi_{\sigma\tau}(v_\circ)\big) \tag{56}$$

and the expectation values $\langle\langle Y(A,z)\rangle\rangle$ of local fields $Y(A,z)$ from the vertex algebra V,

$$\langle\langle Y(A,z)\rangle\rangle \equiv \frac{H(\Psi_{\sigma\tau}(A), \Psi_{\sigma\tau}(A))}{H(\Psi_{\sigma\tau}(v_\circ), \Psi_{\sigma\tau}(v_\circ))}. \tag{57}$$

Following [18] we will regard the partition function $Z_g(X)$ as a hermitian metric $\mathscr{H}$ on the projective line bundle $\mathscr{L}_V$. It follows easily from (10) that

$$\delta_\vartheta \log Z_g(X) = \big\langle\big\langle Y(T[\eta_\vartheta]v_\circ, z)\big\rangle\big\rangle, \tag{58}$$

where $T[\eta] = \sum_{n\in\mathbb{Z}}\eta_n L_n$, δ_ϑ is the derivative corresponding a tangent vector $\vartheta \in T\mathfrak{M}_{g,0}$ and η_ϑ is any element of $\mathbb{C}((t))\partial_t$ which represents ϑ via (9). Equation (58) can be seen as a more precise formulation of the claim from [18] that the expectation value of the stress-energy tensor coincides with the connection on the projective line bundle $\mathscr{L}_V$ which is canonically associated with the metric $\mathscr{H}$. We have thereby reconstructed the main ingredients of the formulation proposed by Friedan and Shenker [18] within the framework provided by the gluing construction.

6 Example of a Nonrational Modular Functor

There is considerable evidence for the claim that the most basic example of a vertex algebra, the Virasoro algebra, yields a realization of the framework above. The results of [35] are essentially equivalent to the construction of the corresponding

modular functor in genus 0. In the following section we shall review the main characteristics of this modular functor.

6.1 Unitary Positive Energy Representations of the Virasoro Algebra

The unitary highest weight representations R_Δ of the Virasoro algebra are labelled by the eigenvalue Δ of the Virasoro generator L_0 on the highest weight vector. It will be convenient to parametrize Δ as follows

$$\Delta_\alpha = \alpha(2\delta - \alpha), \qquad \text{where } c = 1 + 24\delta^2. \tag{59}$$

The representations $R_\alpha \equiv R_{\Delta_\alpha}$ are unitary iff $\Delta \in [0, \infty)$. In terms of the parametrization (59) one may cover this range by assuming that

$$\alpha \in \mathbb{U} \equiv [0, \delta] \cup \left(\delta + i\mathbb{R}^+\right). \tag{60}$$

The representation R_α for $\alpha = 0$ corresponds to the vacuum representation V. The set parametrizes the unitary dual of the Virasoro algebra. In order to indicate an important analogy with the representation theory of noncompact Lie groups we shall call the family of representations R_α with $\alpha \in \delta + i\mathbb{R}^+$ the principal series of representations, which constitute the tempered dual $\mathbb{T}$ of the Virasoro algebra. Pursuing these analogies it seems natural to call the family of representations R_α with $\alpha \in [0, \delta]$ the complementary series.

6.1.1 Free Field Representation

The Fock space $\mathscr{F}$ is defined to be the representation of the commutation relations

$$[\mathsf{a}_n, \mathsf{a}_m] = \frac{n}{2}\delta_{n+m}, \tag{61}$$

which is generated from the vector $\Omega \in \mathscr{F}$ characterised by $a_n\Omega = 0$ for $n > 0$. There is a unique scalar product $(.,.)_{\mathscr{F}}$ on $\mathscr{F}$ such that $\mathsf{a}_n^\dagger = \mathsf{a}_{-n}$ and $(\Omega, \Omega)_{\mathscr{F}} = 1$.

Within $\mathscr{F}$ we may define a one-parameter family of representations $\mathscr{F}_p$ of the Virasoro algebra by means of the formulae

$$\begin{aligned} L_n(p) &= 2(p + in\delta)a_n + \sum_{k\neq 0,n} a_k a_{n-k}, \quad n \neq 0, \\ L_0(p) &= p^2 + \delta^2 + 2\sum_{k>0} a_{-k}a_k. \end{aligned} \tag{62}$$

The representation $\mathscr{F}_p$ is unitary w.r.t. the scalar product $(.,.)_{\mathscr{F}}$ if $p \in \mathbb{R}$. It is furthermore known [13] to be irreducible and therefore isomorphic to R_α if $p = -i(\alpha - \delta)$ for all $\alpha \in \mathbb{U}$.

6.2 Construction of Virasoro Conformal Blocks in Genus Zero

In the case of the Virasoro algebra there exists a unique conformal block G associated to the three punctured sphere which satisfies

$$G(\rho | v_{\alpha_3} \otimes v_{\alpha_2} \otimes v_{\alpha_1}) = 1, \tag{63}$$

v_{α_k}, $k \in \{1, 2, 3\}$ being the highest weight vectors of the representations R_{α_k}, respectively. The corresponding family of operators $\mathsf{Y}^{\alpha_2}_{\alpha_3\alpha_1}(\mathfrak{v}_2|z) : R_{\alpha_1} \to R_{\alpha_3}$ is uniquely characterized by its member corresponding to $\mathfrak{v}_2 = v_{\alpha_2}$, which will be denoted $\mathsf{Y}^{\alpha_2}_{\alpha_3\alpha_1}(z)$.

6.2.1 Free Field Construction of Chiral Vertex Operators

Let us introduce the (left-moving) chiral free field $\varphi(x) = \mathsf{q} + \mathsf{p}x + \varphi_<(x) + \varphi_>(x)$, by means of the expansions

$$\varphi_<(x) = i \sum_{n<0} \frac{1}{n} \mathsf{a}_n e^{-inx}, \qquad \varphi_>(x) = i \sum_{n>0} \frac{1}{n} \mathsf{a}_n e^{-inx}. \tag{64}$$

The operators q and p are postulated to have the following commutation and hermiticity relations

$$[\mathsf{q}, \mathsf{p}] = \frac{i}{2}, \qquad \mathsf{q}^\dagger = \mathsf{q}, \qquad \mathsf{p}^\dagger = \mathsf{p}, \tag{65}$$

which are naturally realized in the Hilbert-space

$$\mathfrak{H}^{\mathrm{F}} \equiv L^2(\mathbb{R}) \otimes \mathscr{F}. \tag{66}$$

Diagonalizing the operator p corresponds to decomposing $\mathfrak{H}^{\mathrm{F}}$ as direct integral of irreducible unitary representations of the Virasoro algebra,

$$\mathscr{M} \simeq \int_{\mathbb{T}}^{\oplus} d\alpha R_\alpha. \tag{67}$$

The basic building blocks of all constructions will be the following objects:

NORMAL ORDERED EXPONENTIALS:

$$\mathsf{E}^\alpha(x) \equiv \mathsf{E}^\alpha_<(x)\mathsf{E}^\alpha_>(x), \qquad \begin{aligned} \mathsf{E}^\alpha_<(x) &= e^{\alpha\mathsf{q}} e^{2\alpha\varphi^+_<(x)} e^{\alpha x\mathsf{p}} \\ \mathsf{E}^\alpha_>(x) &= e^{\alpha x\mathsf{p}} e^{2\alpha\varphi^+_>(x)} e^{\alpha\mathsf{q}}. \end{aligned} \tag{68}$$

SCREENING CHARGES:

$$\mathsf{Q}(x) \equiv e^{-\pi b\mathsf{p}} \int_0^{2\pi} dx' \mathsf{E}^b(x+x') e^{-\pi b\mathsf{p}}. \tag{69}$$

The following property is of considerable importance:

POSITIVITY: The screening charges are densely defined positive operators, i.e.

$$\big(\psi, Q(\sigma)\psi\big)_{\mathscr{M}} \geq 0$$

holds for ψ taken from a dense subset of $\mathfrak{H}$.

Out of the building blocks introduced in the previous subsection we may now construct an important class of chiral fields,

$$\mathsf{h}_s^\alpha(\sigma) = \mathsf{E}^\alpha(\sigma)\big(\mathsf{Q}(\sigma)\big)^s. \tag{70}$$

Positivity of Q allows us to consider these objects for *complex* values of s and α.

One of the most basic properties of the $\mathsf{h}_s^\alpha(w)$ are the simple commutation relations with functions of the operator p,

$$\mathsf{h}_s^\alpha(w) f(\mathsf{p}) = f\big(\mathsf{p} - i(\alpha + bs)\big)\mathsf{h}_s^\alpha(w). \tag{71}$$

By projecting onto eigenspaces of p one may therefore define a family of operators $\mathsf{h}^{\alpha_2}_{\alpha_3\alpha_1}(w) : R_{\alpha_1} \to R_{\alpha_3}$. Specifically, for each $\mathfrak{w} \in \mathscr{F}$ and each $\alpha \in \delta + i\mathbb{R}$ let us define a distribution $\mathfrak{w}_\alpha$ on dense subspaces of $\mathscr{M}$ by the relation $(\mathfrak{w}_\alpha, \mathfrak{v})_{\mathscr{M}} = (\mathfrak{w}, \mathfrak{v}_\alpha)_{\mathscr{F}}$ if $\mathfrak{v}$ is represented via (67) by the family of vectors $\mathfrak{v}_\alpha$, $\mathfrak{v}_\alpha \in R_\alpha$. This implies that the matrix elements of the operators $\mathsf{h}^{\alpha_2}_{\alpha_3\alpha_1}(w)$ are determined by the relation

$$\big(\mathfrak{w}, \mathsf{h}^{\alpha_2}_{\alpha_3\alpha_1}(w)\mathfrak{u}\big)_{\mathscr{F}} = \big(\mathfrak{w}_{\alpha_3}, \mathsf{h}_s^{\alpha_2}(w)\hat{\mathfrak{u}}\big)_{\mathscr{M}}, \tag{72}$$

where $bs = \alpha_3 - \alpha_1 - \alpha_2$ and $\hat{\mathfrak{u}}$ is any vector in $\mathscr{M}$ represented by the family of vectors $\hat{\mathfrak{u}}_\alpha$ such that $\hat{\mathfrak{u}}_{\alpha_1} = \mathfrak{u}$.

The uniqueness of the conformal block $G^{(3)}$ implies that the operator $\mathsf{Y}^{\alpha_2}_{\alpha_3\alpha_1}(\mathfrak{v}_2|z)$ must be proportional to $\mathsf{h}^{\alpha_2}_{\alpha_3\alpha_1}(\mathfrak{v}_2|z)$ via

$$\mathsf{Y}^{\alpha_2}_{\alpha_3\alpha_1}(\mathfrak{v}_2|z) = N^{\alpha_2}_{\alpha_3\alpha_1}\mathsf{h}^{\alpha_2}_{\alpha_3\alpha_1}(\mathfrak{v}_2|z). \tag{73}$$

The explicit formula for the normalizing factor $N^{\alpha_2}_{\alpha_3\alpha_1}$ was found in [35].

6.3 Factorization Property

The results of [35] show that the conformal blocks in genus zero satisfy the factorization property with linear relations (37) composed from the elementary transformations F_{pq}, B_p and Z_p whose representatives can be calculated explicitly.

F: Let X be a four-punctured sphere and let σ_s, σ_u be the two markings depicted in Fig. 7. We will denote the respective assignments of representation labels to the edges of σ_s and σ_u by $\rho_s(\alpha_s)$ and $\rho_u(\alpha_u)$, respectively, leaving implicit the assignment of labels $\alpha_1, \alpha_2, \alpha_3, \alpha_4$ to the external edges with numbering being indicated in Fig. 7. The operator $\mathbf{F}_{pq}$ may then be represented as the integral operator

$$G_{\sigma_s\tau_2}(\rho_s(\alpha_s)) = \int d\mu_{\rm Pl}(\alpha_u) \mathrm{F}_{\alpha_s\alpha_u}\left[\begin{matrix}\alpha_3 & \alpha_2\\ \alpha_4 & \alpha_1\end{matrix}\right] G_{\sigma_u\tau_1}(\rho_u(\alpha_u)). \tag{74}$$

The explicit expression for the kernel $\mathrm{F}_{\alpha_s\alpha_u}\left[\begin{smallmatrix}\alpha_3 & \alpha_2\\ \alpha_4 & \alpha_1\end{smallmatrix}\right]$ can be found in [34, 35]. More illuminating is probably the observation that the kernel $\mathrm{F}_{\alpha_s\alpha_u}$ is closely related to the $6j$ symbols [27] of the modular double [6, 4] of $\mathscr{U}_q(\mathfrak{sl}(2,\mathbb{R}))$,

$$\mathrm{F}_{\alpha_s\alpha_u}\left[\begin{matrix}\alpha_3 & \alpha_2\\ \alpha_4 & \alpha_1\end{matrix}\right] = \frac{\nu^{\alpha_4}_{\alpha_3\alpha_s}\nu^{\alpha_s}_{\alpha_2\alpha_1}}{\nu^{\alpha_4}_{\alpha_u\alpha_1}\nu^{\alpha_u}_{\alpha_3\alpha_2}}\left\{\begin{matrix}\alpha_1 & \alpha_2\\ \alpha_3 & \alpha_4\end{matrix}\middle|\begin{matrix}\alpha_s\\ \alpha_u\end{matrix}\right\}. \tag{75}$$

The explicit formula for the normalizing factors $\nu^{\alpha_s}_{\alpha_2\alpha_1}$ can be found in [34].

B: Let X be a three-punctured sphere and let σ_2, σ_1 be the two markings depicted on the left and right halves of Fig. 2, respectively. Let ρ be the assignment $\rho : k \to \alpha_k$, $k = 1, 2, 3$ of representation labels to edges as numbered in Fig. 2. We then have

$$G_{\sigma_2}(\rho) = \mathrm{B}_{\alpha_3\alpha_2\alpha_1} G_{\sigma_1}(\rho), \qquad \mathrm{B}_{\alpha_3\alpha_2\alpha_1} \equiv e^{\pi i(\alpha_3(Q-\alpha_3)-\alpha_1(Q-\alpha_1)-\alpha_2(Q-\alpha_2))}. \tag{76}$$

Z: Z is represented by the identity operator.

An important part of the statements above may be reformulated as the claim that the modular functor $\mathscr{F}_{\rm Teich}$ is similar in the sense of Definition 9 to a modular functor $\mathscr{F}_{\rm Qgrp}$ that is constructed in close analogy to the construction of Reshetikhin-Turaev from the representations of the modular double of $\mathscr{U}_q(\mathfrak{sl}(2,\mathbb{R}))$ introduced in [28, 6] and studied in more detail in [28, 4].

6.4 The Hilbert Space Structure

As explained above, we need a pair $\left[\mathfrak{H}^{(3)}_\sigma(\rho), d\mu_{\rm Pl}\right]$ of objects in order to characterize the Hilbert space structures on the spaces of conformal blocks.

Hilbert space $\mathfrak{H}^{(3)}_\sigma(\rho)$: It is well-known that the space of conformal blocks on the three punctured sphere is at most one-dimensional. More precisely we have:

$$\mathfrak{H}^{(3)}_\sigma(\rho) \simeq \mathbb{C}, \qquad \rho : k \mapsto \alpha_k, k \in \{1, 2, 3\}, \tag{77}$$

if $\alpha_i \neq 0$ for $i = 1, 2, 3$. If $\alpha_i = 0$ for some $i \in \{1, 2, 3\}$ and if $k, l \in \{1, 2, 3\}$ are not equal to i we have

$$\mathfrak{H}_\sigma^{(3)}(\rho) \simeq \begin{cases} \mathbb{C} & \text{if } \alpha_k = \alpha_l \text{ or } \alpha_k = 2\delta - \alpha_l, \\ \emptyset & \text{otherwise.} \end{cases} \tag{78}$$

As a standard basis for $\mathfrak{H}_\sigma^{(3)}(\rho)$ we shall use the conformal block $G^{(3)}(\rho)$ that is uniquely defined by the normalization (63). The Hilbert space structure on the one-dimensional space $\mathfrak{H}_s i^{(3)}(\rho)$ is then described by the numbers

$$D(\alpha_3, \alpha_2, \alpha_1) \equiv \|G^{(3)}(\rho)\|^2, \tag{79}$$

that are given explicitly by the formula

$$D(\alpha_3, \alpha_2, \alpha_1) = \left| \frac{\Gamma_b(\alpha_{123} - Q)}{\Gamma_b(Q)} \prod_{k=1}^{3} \frac{\Gamma_b(\alpha_{123} - 2\alpha_k)}{\Gamma_b(2\alpha_k)} \right|^2, \tag{80}$$

where $\Gamma_b(x) \equiv \Gamma_2(x|b, b^{-1})$ with $\Gamma_2(x|\omega_1, \omega_2)$ being the Barnes Double Gamma function, and we have used the abbreviation $\alpha_{123} = \alpha_1 + \alpha_2 + \alpha_3$.

The measure $d\mu_{\rm Pl}$ on $\mathbb{U}$ will then be equal to

$$d\mu_{\rm Pl}(\alpha) = d\alpha \sin(2b(\alpha - \delta)) \sin(2b^{-1}(\delta - \alpha)) \quad \text{on } \delta + i\mathbb{R}^+, \tag{81}$$

with $d\alpha$ being the standard Lebesque measure on $\delta + i\mathbb{R}^+$.

6.5 Extension to Higher Genus

Claim. There exists a unique extension of the $g = 0$ modular functor $\mathscr{F}_{\rm Vir}$ to $g > 0$ that is compatible with the propagation of vacua.

The proof of this claim has not appeared in the literature yet. Let us therefore briefly sketch the path along which the author has arrived at the claim above.

The main observation to be made is that there exists a unitary modular functor $\mathscr{F}_{\rm Teich}$ whose restriction to $g = 0$ is similar to $\mathscr{F}_{\rm Vir}$ in the sense of Definition 9. $\mathscr{F}_{\rm Teich}$ was constructed in [36].[8]

Uniqueness is in fact quite easily seen by noting that arguments well-known from rational conformal field theory [25] carry over to the case at hand and allow us to derive an explicit formula for the coefficients $S_{\alpha\beta}(\gamma)$ in terms of $\mathrm{F}_{\alpha_s\alpha_u}\left[\begin{smallmatrix}\alpha_3 & \alpha_2\\ \alpha_4 & \alpha_1\end{smallmatrix}\right]$ and $\mathrm{B}_{\alpha_3\alpha_2\alpha_1}$, namely

[8] The key step in the verification of our claim above is to notice that the restriction of $\mathscr{F}_{\rm Teich}$ to surfaces with $g = 0$ is similar to the modular functor $\mathscr{F}_{\rm Qgrp}^{g=0}$ coming from the harmonic analysis on the modular double of $\mathscr{U}_q(\mathfrak{sl}(2, \mathbb{R}))$ that was mentioned above. This establishes the existence of an extension of $\mathscr{F}_{\rm Vir}$ to $g > 0$.

$$F_{0\beta}\begin{bmatrix}\alpha_1 & \alpha_1\\ \alpha_1 & \alpha_1\end{bmatrix} S_{\alpha_1\alpha_2}(\beta)$$
$$= S_{0\alpha_2}(0)\int d\mu_{\mathrm{PL}}(\gamma)e^{\pi i(2\Delta_{\alpha_2}+2\Delta_{\alpha_1}-2\Delta_\gamma-\Delta_\beta)}\mathrm{F}_{0\gamma}\begin{bmatrix}\alpha_2 & \alpha_1\\ \alpha_2 & \alpha_1\end{bmatrix}\mathrm{F}_{\gamma\beta}\begin{bmatrix}\alpha_1 & \alpha_1\\ \alpha_2 & \alpha_2\end{bmatrix}. \tag{82}$$

6.6 Remarks

It is often natural to first focus attention on the subspace of "tempered" conformal blocks which are obtained from the gluing construction by using three point conformal blocks associated to representations from the tempered dual $\mathbb{T}$ only. The formulation of the theory as a modular functor applies straightforwardly to this case.

However, in the case of the Virasoro algebra we may observe rather nice analytic properties of the conformal blocks when considered as functions of the representation labels α_k [34]. The dependence w.r.t. the external representations is *entire analytic*, while the dependence w.r.t. the internal representations is *meromorphic*. The poles are given by the zeros of the Kac determinant.

The factorization property of the analytically continued conformal blocks follows from the corresponding property of the tempered conformal blocks. Analytic continuation w.r.t. the representation labels therefore allows us to generate a large class of conformal blocks with reasonable behavior at the boundaries of the Teichmüller spaces from the tempered conformal blocks. We will call this class of conformal blocks the factorizable conformal blocks. It is not clear to the author how this class compares to the set of *all* solutions to the conformal Ward identities.

7 Existence of a Canonical Scalar Product?

We propose that for each vertex algebra V whose conformal blocks have the factorization property there always exists a distinguished choice for H_σ, canonically associated to V, which is "diagonal", i.e. such that H_σ is of the form

$$H_\sigma = \int_{\mathbb{U}^{\sigma_1}} \prod_{e\in\sigma_1} d\mu_{\mathrm{Pl}}(r_e) \bigotimes_{p\in\sigma_0} H_p^{\bar\rho_p\rho_p}, \tag{83}$$

where $\bar\rho_p$ is the decoration of S_p obtained from ρ_p by replacing each representation by its dual, σ_1 is the set of edges and σ_0 is the set of vertices of the graph σ. In rational CFT this case is often referred to as the CFT corresponding to the "diagonal modular invariant". We propose the terminology "V-minimal model" for the corresponding CFT.

Whenever the hermitian form H is positive definite we get a *scalar product* on the space of conformal blocks. We will subsequently argue that this is always the case if the representations in question are unitary.

7.1 Existence of a Canonical Hermitian Form from the Factorization Property

Note that $\dim \mathfrak{H}^{r_3}_{r_2 r_1} = 1$ whenever one of the representations R_{r_i}, $i = 1, 2, 3$ coincides with the vacuum representation, and the two other representations are R and $\bar{R}$, with $\bar{R}$ being the dual of R. This implies that there is a unique (up to a constant) conformal block associated to the diagram on the left of Fig. 9 if the representation associated to the edges with label 0 is the vacuum representation and if the representations associated to the edges with labels $1, \bar{1}, 2, \bar{2}$ are chosen as $R_1, \bar{R}_1, R_2, \bar{R}_2$, respectively. This conformal block will be denoted as $G^{\sigma_1}_{\mathrm{o}\tau}\left[\begin{smallmatrix} r_2 & \bar{r}_1 \\ \bar{r}_2 & r_1 \end{smallmatrix}\right]$.

Let us, on the other hand, use the notation $G^{\sigma_2}_{r_3\tau}\left[\begin{smallmatrix} \bar{r}_2 & r_2 \\ \bar{r}_1 & r_1 \end{smallmatrix}\right]_{\iota\bar{\iota}}$ for the conformal blocks associated to the diagram on the right of Fig. 9 in the case that the representations associated to the edges with labels $1, 2, \bar{1}, \bar{2}$ are chosen as above. The indices $\iota, \bar{\iota}$ are associated to the vertices enclosed in little circles in a manner that should be obvious.

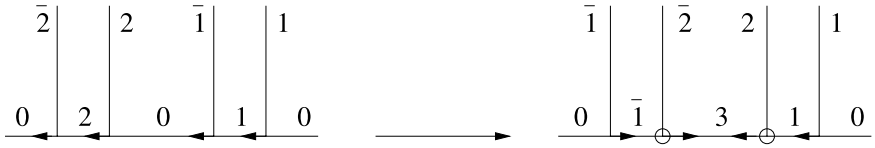

Fig. 9 Simplified representation for the markings involved in the relation (84)

Bear in mind that we are considering vertex algebras whose conformal blocks have the factorization property. It follows in particular that the conformal blocks $G^{\sigma_1}_{\mathrm{o}\tau}\left[\begin{smallmatrix} r_2 & \bar{r}_1 \\ \bar{r}_2 & r_1 \end{smallmatrix}\right]$ and $G^{\sigma_2}_{r_3\tau}\left[\begin{smallmatrix} \bar{r}_2 & r_2 \\ \bar{r}_1 & r_1 \end{smallmatrix}\right]_{\bar{\iota}\iota}$ are related by an expansion of the form

$$G^{\sigma_1}_{\mathrm{o}\tau}\begin{bmatrix} r_2 & \bar{r}_1 \\ \bar{r}_2 & r_1 \end{bmatrix} = \int d\mu_{12}(r_3) \sum_{\iota,\bar{\iota}\in\mathbb{I}_p} D_{\bar{\iota}\iota}(r_3|r_2, r_1) G^{\sigma_2}_{r_3\tau}\begin{bmatrix} \bar{r}_2 & r_2 \\ \bar{r}_1 & r_1 \end{bmatrix}_{\bar{\iota}\iota}. \tag{84}$$

Conjecture 10 *There exists a subset $\mathbb{T}$ of $\mathbb{U}$ parameterizing "tempered" representations such that for $r_1, r_2 \in \mathbb{T}$ the measure $d\mu_{12}$ is supported in $\mathbb{T}$. In this case there exists a factorization of the form*

$$d\mu_{12}(r_3) D_{\iota\bar{\iota}}(r_3|r_2, r_1) = d\mu_{\mathrm{Pl}}(r_3) D_{\bar{\iota}\iota}(r_3, r_2, r_1), \tag{85}$$

with $d\mu_{\mathrm{Pl}}$ being independent of r_2, r_1 such that the hermitian forms on spaces of conformal blocks constructed via (83) *from $d\mu_{\mathrm{Pl}}(s)$ and $D_{\bar{\imath}\imath}(r_3, r_2, r_1)$*[9] *satisfy the invariance property* (39).

In other words, the data appearing in the relationship (84) characterize a hermitian form on spaces of conformal blocks canonically associated with any vertex algebra V that has the factorization property.

7.1.1

Let us note that validity of the conjecture above is known in the case of rational CFT's. Indeed, let us keep in mind that according to Sect. 3.3.2 above one may express the three point function in the V-minimal model in terms of the numbers $D_{\imath\bar{\imath}}(r_3, r_2, r_1)$ introduced in the conjecture above. In the case that the operators Z_p, B_p and F_{pq} are represented by matrices it is easy to figure out an expression of $D_{\imath\bar{\imath}}(r_3, r_2, r_1)$ in terms of the matrix elements of Z_p and F_{pq}. This expression coincides with the formula for the three point function that was obtained as a special case of the general formalism developed in [32] for the description of correlation function in rational CFT. Invariance of the corresponding hermitian form follows from the relations satisfied by the operators Z_p, B_p F_{pq}, S_p that were discussed in the previous section.

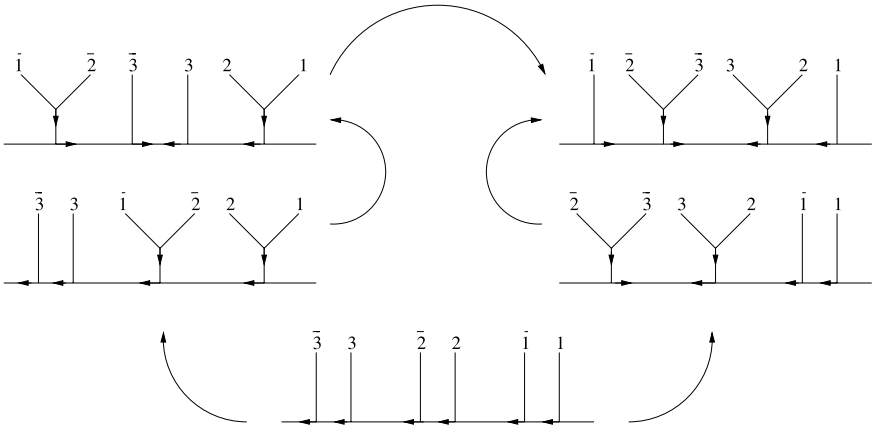

Fig. 10 Proof of invariance under F

Our main point is of course to propose that a similar relationship also holds in nonrational cases. And indeed, given that there exists a factorization of the form (85) it is not hard to show invariance under F by considering the sequence of transformations indicated in Fig. 10. Invariance under B is verified similarly. Invariance under

[9] $H_p^{\tilde{\rho}\rho}(f, g) = \sum_{\bar{\imath},\imath\in\mathbb{I}} (f(\imath'))^* D_{\bar{\imath}\imath}(r_3, r_2, r_1) g(\imath)$.

Z follows from the invariance under F thanks to (40). The conjecture is furthermore supported by the results from [35] reviewed in Sect. 6 above.

7.2 Unitary Fusion

There is a generalization of the tensor product for unitary representations of certain vertex algebras that has the virtue to make unitarity of the resulting representation manifest. The underlying theory is closely related to the theory of superselection sectors from algebraic quantum field theory [12, 19]. We will in the following briefly discuss a reformulation called "Connes-fusion" [38].

In order to simplify the exposition, we will restrict attention to the case of the Virasoro algebra with $c > 25$. What follows is a sketch of the picture that would result from using the results of [35] within a theory of "Connes-fusion" of representations of $\mathrm{Diff}(S_1)$ along the lines of [38]. The author believes that similar things can be done for many other vertex algebras, which would allow one to show that the canonical hermitian form proposed in the previous subsection is positive definite in the case of unitary representations.

7.2.1

It is temporarily useful to replace the states v_m within the representations R_m, $m = 1, 2$ by the vertex operators $\mathsf{V}_m \equiv \mathsf{V}_m(v_m)$ which generate the states v_m from the vacuum, $v_m = \mathsf{V}_m\Omega$. We want to think of representations R_m, $m = 1, 2$ as representations of $\mathrm{Diff}(\mathrm{I}_m)$ associated to the intervals $\mathrm{I}_m \subset S_1$, $\mathrm{I}_1 \cup \mathrm{I}_2 = S_1$, respectively. The vertex operators V_m should therefore commute with the action of $\mathrm{Diff}(\mathrm{I}_m^c)$, $\mathrm{I}_m^c = S_1 \setminus \mathrm{I}_m$ as

$$\pi_{R_m}(g)\mathsf{V}_m = \mathsf{V}_m\pi_{\mathfrak{o}}(g) \quad \text{for all} \quad g \in \mathrm{Diff}(\mathrm{I}_m^c), \tag{86}$$

with $\pi_{\mathfrak{o}}(g)$ being the action of $\mathrm{Diff}(\mathrm{I}_m^c)$ on the vacuum representation V. Operators with such a property can be constructed from the chiral vertex operators $\mathsf{Y}^{\alpha_2}_{\alpha_3\alpha_1}(\mathfrak{v}_2|z)$ as

$$\mathsf{V}_m \equiv \int_{\mathrm{I}_m} dx f_m(x)\mathsf{Y}^{r_m}_{r_m 0}(\mathfrak{v}_m|e^{ix}), \qquad m = 1, 2, \tag{87}$$

f being a smooth function with support in I_m. Operators like the one defined in (87) will be unbounded in general, but bounded operators can be obtained by taking the phase of its polar decomposition.

Let us then consider the spaces $\mathscr{V}_m$ of *bounded* intertwiners $\mathsf{V}_m : V \to R_m$ which satisfy (86). On $\mathscr{V}_1 \otimes \mathscr{V}_2$ define an inner product by

$$\left\langle w_1 \otimes w_2, v_1 \otimes v_2 \right\rangle = \left\langle \Omega, \mathsf{W}_2^*\mathsf{V}_2.\mathsf{W}_1^*\mathsf{V}_1\Omega \right\rangle. \tag{88}$$

The Hilbert space completion of $\mathscr{V}_1 \otimes \mathscr{V}_2$ is denoted $R_1 \boxtimes R_2$. We observe that the scalar product of the "fused" representation is defined in terms of the conformal block $G_{\sigma\tau}^{\sigma_1}\left[\begin{smallmatrix} r_2 & \tilde{r}_1 \\ \tilde{r}_2 & r_1 \end{smallmatrix}\right]$ that had previously appeared in the relations (84).

7.2.2

In the case of the Virasoro algebra one may deduce the validity of relations (84) from (74) by analytically continuing α_s to the value $\alpha_s = 0$. This allows one to write $\|v_1 \otimes v_2\|^2$ in the form

$$\|v_1 \otimes v_2\|^2 = \int_{\mathbb{U}} d\mu_{21}(\alpha_s) \|\mathsf{V}_{\alpha_s}^{(2)}(v_2, v_1)\|_{R_{\alpha_s}}^2, \tag{89}$$

where $\mathsf{V}_{\alpha_s}^{(2)}(v_2, v_1)$ is a certain vector in the *irreducible* representation R_{α_s} that may be written as

$$\mathsf{V}_{\alpha_s}^{(2)}(v_2, v_1) \equiv \mathsf{V}_{s1}^2 v_1 = \int_{\mathrm{I}_2} dx f_2(x) \mathsf{Y}_{\alpha_s \alpha_1}^{\alpha_2}(\mathfrak{v}_2 | e^{ix}) \mathsf{V}_1 \Omega,$$

provided that V_2 can be represented in the form (87). Note that the space $R_1 \boxtimes R_2$ is naturally a representation of $\mathrm{Diff}(\mathrm{I}_1) \times \mathrm{Diff}(\mathrm{I}_2)$. Equation (89) is interpreted as an expression for the unitary equivalence

$$R_1 \boxtimes R_2 \simeq \int_{\mathbb{U}}^{\oplus} d\mu_{21}(s) R_s \tag{90}$$

which implies in particular the fact that the representation of $\mathrm{Diff}(\mathrm{I}_1) \times \mathrm{Diff}(\mathrm{I}_2)$ on $R_1 \boxtimes R_2$ can be extended to a representation of $\mathrm{Diff}(S^1)$. The factorization $d\mu_{21}(s) = d\mu_{\mathrm{Pl}}(s) D(r_3, r_2, r_1)$ then allows us to rewrite (90) as

$$R_1 \boxtimes R_2 \simeq \int_{\mathbb{U}}^{\oplus} d\mu_{\mathrm{Pl}}(s) R_s \otimes \mathrm{Hom}(R_1 \boxtimes R_2; R_s), \tag{91}$$

where $\mathrm{Hom}(R_1 \boxtimes R_2; R_s)$ is the one-dimensional Hilbert space of intertwiners with metric given by $D(r_3, r_2, r_1)$.

7.3 Associativity of Unitary Fusion

It should be possible to show on general grounds that the fusion operation is associative,

$$(R_1 \boxtimes R_2) \boxtimes R_3 \equiv R_1 \boxtimes R_2 \boxtimes R_3 \equiv R_1 \boxtimes (R_2 \boxtimes R_3). \tag{92}$$

Indeed, let us consider

$$\|(v_1 \otimes v_2) \otimes v_3\|^2 \quad \text{and} \quad \|v_1 \otimes (v_2 \otimes v_3)\|^2. \tag{93}$$

The left hand side and the right hand side of (93) can be represented respectively as

$$\int_{\mathbb{U}} d\mu_{12}(\alpha_s)\big\langle \Omega, \mathsf{V}_3^* \mathsf{V}_3 \mathsf{V}_{21}^*(\alpha_s)\mathsf{V}_{21}(\alpha_s)\Omega\big\rangle, \qquad \mathsf{V}_{21}(\alpha_s) \equiv \mathsf{V}_{s1}^2 \mathsf{V}_1, \tag{94}$$

$$\int_{\mathbb{U}} d\mu_{23}(\alpha_u)\big\langle \Omega, \mathsf{V}_{32}^*(\alpha_u)\mathsf{V}_{32}(\alpha_u)\mathsf{V}_1^* \mathsf{V}_1 \Omega\big\rangle, \qquad \mathsf{V}_{32}(\alpha_u) \equiv \mathsf{V}_{u2}^3 \mathsf{V}_2. \tag{95}$$

It is useful to note that the compositions of chiral vertex operators which appear in (94) and (95) correspond to the diagrams on the left and right in the middle line of Fig. 10, respectively. From this diagrammatic representation it is easily seen that (94) and (95) are both equal to

$$\langle \Omega, \mathsf{V}_3^* \mathsf{V}_3 \mathsf{V}_2^* \mathsf{V}_2 \mathsf{V}_1^* \mathsf{V}_1 \Omega\rangle \equiv \|v_1 \otimes v_2 \otimes v_3\|^2, \tag{96}$$

corresponding to the diagram on the bottom of Fig. 10, which makes the associativity of the fusion operation manifest. By using (89) one may rewrite (94) and (95) respectively in the form

$$\begin{aligned} &\int_{\mathbb{U}} d\mu_{123}(\alpha_4)\big\|\mathsf{V}^{(3)}_{\alpha_4,s}(v_3, v_2, v_1)\big\|^2, \\ &\mathsf{V}^{(3)}_{\alpha_4,s}(v_3, v_2, v_1) \equiv \int_{\mathbb{U}} d\mu_{12}(\alpha_s)\mathsf{V}^{(2)}_{\alpha_4}(v_3, \mathsf{V}^{(2)}_{\alpha_s}(v_2, v_1)) \end{aligned} \tag{97}$$

$$\begin{aligned} &\int_{\mathbb{U}} d\mu_{123}(\alpha_4)\big\|\mathsf{V}^{(3)}_{\alpha_4,u}(v_3, v_2, v_1)\big\|^2, \\ &\mathsf{V}^{(3)}_{\alpha_4,u}(v_3, v_2, v_1) \equiv \int_{\mathbb{U}} d\mu_{23}(\alpha_u)\mathsf{V}^{(2)}_{\alpha_4}(\mathsf{V}^{(2)}_{\alpha_u}(v_3, v_2), v_1). \end{aligned} \tag{98}$$

These relations may both be seen as expressions for the unitary equivalences

$$(R_1 \boxtimes R_2) \boxtimes R_3 \simeq \int_{\mathbb{U}}^{\oplus} d\mu_{\mathrm{Pl}}(\alpha) R_\alpha \otimes L^2(\mathbb{U}, d\mu^{\alpha}_{(12)3}), \tag{99}$$

$$R_1 \boxtimes (R_2 \boxtimes R_3) \simeq \int_{\mathbb{U}}^{\oplus} d\mu_{\mathrm{Pl}}(\alpha) R_\alpha \otimes L^2(\mathbb{U}, d\mu^{\alpha}_{1(23)}), \tag{100}$$

where

$$\begin{aligned} d\mu^{\alpha}_{(12)3}(\alpha_s) &= d\mu_{\mathrm{Pl}}(\alpha_s) D(\alpha_s, \alpha_2, \alpha_1) D(\alpha, \alpha_3, \alpha_s) \\ d\mu^{\alpha}_{1(23)}(\alpha_u) &= d\mu_{\mathrm{Pl}}(\alpha_u) D(\alpha_u, \alpha_3, \alpha_2) D(\alpha, \alpha_u, \alpha_1). \end{aligned}$$

It should be noted that the Hilbert spaces $L^2(\mathbb{U}, d\mu^{\alpha}_{(12)3})$ and $L^2(\mathbb{U}, d\mu^{\alpha}_{1(23)})$ which appear in (99) and (100), respectively, are nothing but different models for Hilbert-subspaces of $\mathrm{Hom}(R_1 \boxtimes R_2 \boxtimes R_3; R_\alpha)$. These Hilbert spaces are canonically isomorphic to the spaces of conformal blocks $\mathscr{H}_{\sigma_1}$ and $\mathscr{H}_{\sigma_2}$ associated to the markings on the left and right of Fig. 7, respectively. It therefore follows from the associativity of the fusion product that there exists a one-parameter family of unitary operators

$\mathsf{F} : \mathscr{H}_{\sigma_1} \to \mathscr{H}_{\sigma_2}$ that represents the unitary equivalence between the representations (99) and (100), respectively.

7.4 Discussion

The author believes that the link between the hermitian form on spaces of conformal blocks and unitary fusion has not received the attention it deserves. More specifically, there are two reasons why the authors believes that the connection between the unitary fusion and the hermitian form on spaces of conformal blocks is worth noting and being better understood:

On the one hand, it offers an explanation for the positivity of the coefficients $D_{i\bar{\imath}}(r_3, r_2, r_1)$ defining the hermitian form H_V in the unitary case, thereby elevating it to a scalar product.

If, on the other hand, one was able to show on a priori grounds that the representation $\mathrm{Diff}(\mathrm{I}_1) \times \mathrm{Diff}(\mathrm{I}_2)$ on $R_1 \boxtimes R_2$ can be extended to a representation of $\mathrm{Diff}(S^1)$ then one might use this as a basis for a conceptual proof of the factorization property (37) in genus 0 along the lines sketched above.

It does not seem to be possible, however, to give a simple explanation of the factorization (85) in Conjecture 10 from this point of view. This deep property seems to require new ideas for its explanation. We see it as a hint towards an even deeper level of understanding CFT in its relation to the harmonic analysis of $\mathrm{Diff}(S_1)$, or some extension thereof.

8 Outlook

First we would like to stress that the class of nonrational CFT covered by the formalism described in this paper is expected to contain many CFTs of interest. To illustrate this claim, let us formulate the following conjecture.

8.1 Modular Functors from W-algebras and Langlands Duality

We would finally like to formulate a conjecture. Let $W_k(\mathfrak{g})$ be the W-algebra constructed in [7, 8]

Conjecture 11 *There exists a family of stable unitary modular functors*

$$\big(\Sigma, \mathfrak{g}, k\big) \longmapsto \big(\mathfrak{H}_{\mathfrak{g},k}(\Sigma), \mathsf{M}_{\mathfrak{g},k}(\Sigma)\big)$$

that is canonically isomorphic to either

> *the space of conformal blocks for certain classes of unitary representations of the W-algebra $\mathscr{W}_k(\mathfrak{g})$ with its natural unitary mapping class group action,*

or

> *the space of states obtained via the quantization of the higher Teichmüller spaces* [10, 11] *together with its canonical mapping class group action*

such that Langlands duality holds: There is a canonical isomorphism

$$\big(\mathfrak{H}_{\mathfrak{g},k}(\Sigma), \mathsf{M}_{\mathfrak{g},k}(\Sigma)\big) \simeq \big(\mathfrak{H}_{{}^{\mathrm{L}}\mathfrak{g},\check{k}}(\Sigma), \mathsf{M}_{{}^{\mathrm{L}}\mathfrak{g},\check{k}}(\Sigma)\big),$$

with ${}^{\mathrm{L}}\mathfrak{g}$ *being the Langlands dual to the Lie algebra* $\mathfrak{g}$ *and* $\check{k}$ *being related to* k *via* $(k+h^\vee)r^\vee = (\check{k}+h^\vee)^{-1}$, $h^\vee$ *being the dual Coxeter number.*

8.2 Boundary CFT

It seems interesting to note a link to boundary CFT. In the case of the V-minimal model one expects following Cardy's analysis [5] to find a one-to-one correspondence between conformal boundary conditions and irreducible representations. There should in particular exist a distinguished boundary condition $B_{\mathfrak{o}}$ which corresponds to the vacuum representation.

This boundary condition is fully characterized by the measure appearing in the expansion of the corresponding boundary state into the Ishibashi-states $|r\rangle\rangle$ which preserve the full chiral algebra V,

$$|B_{\mathfrak{o}}\rangle = \int_{\mathbb{U}} d\mu_{\mathrm{B}_{\mathfrak{o}}}(r)|r\rangle\rangle. \tag{101}$$

It is not hard to see that the two-point function $\langle V_2(z_2,\bar{z}_2)V_1(z_1,\bar{z}_1)\rangle_{B_{\mathfrak{o}}}$ in the presence of a boundary with condition $B_{\mathfrak{o}}$ is proportional to $G^{\sigma_1}_{\mathfrak{o}\tau}\left[\begin{smallmatrix} r_2 & \bar{r}_1 \\ \bar{r}_2 & r_1 \end{smallmatrix}\right]$. The expansion (84) describes the OPE of the two fields V_1, V_2. It easily follows from these observations that the one-point function (in a suitable normalization) coincides with the Plancherel-measure $d\mu_{\mathrm{Pl}}(s)$,

$$d\mu_{\mathrm{B}_{\mathfrak{o}}}(r) = d\mu_{\mathrm{Pl}}(r). \tag{102}$$

We take this observation as an intriguing hint concerning the generalization of our considerations to boundary CFT.

8.3 Nonrational Verlinde Formula?

In the case of rational CFT one can deduce a lot of useful relations [24, 25] between the defining data of a modular functor from the relations (28)–(30), (35)–(36) and (40)–(43). These relations give the key to some derivations of the famous Verlinde formula. Much of this remains intact in the nonrational case, as the example of formula (82) illustrates.

A fundamental difference comes from the fact that the vacuum representation is *not* in the support of μ_{Pl}. This implies that objects like $\mathrm{F}_{\alpha\beta}\left[\begin{smallmatrix}\alpha_3 & \alpha_2\\ \alpha_4 & \alpha_1\end{smallmatrix}\right]$ or $S_{\alpha\beta}(\gamma)$ are not necessarily well-defined at $\beta = 0$. This means that many of the relations valid in rational CFT do not have obvious counterparts in the nonrational case.

As a particularly interesting example let us note that in the case of the minimal models one has the relation [31]

$$\mathrm{F}_{0r}\begin{bmatrix} r_2 & r_1\\ r_2 & r_1\end{bmatrix}\mathrm{F}_{r0}\begin{bmatrix} r_2 & r_2\\ r_1 & r_1\end{bmatrix} = \frac{S_{0r}S_{00}}{S_{0r_2}S_{0r_1}}, \qquad S_{r_1r_2} \equiv S_{r_1r_2}(0). \tag{103}$$

As explained above, the left hand side does not have an obvious counterpart in the nonrational case in general. However, in the case of the Virasoro algebra with $c > 25$ it turns out that

$$\mathrm{F}''_{\alpha 0}\begin{bmatrix} \alpha_3 & \alpha_2\\ \alpha_4 & \alpha_1\end{bmatrix} = \lim_{\beta\to 0}\beta^2\mathrm{F}_{\alpha\beta}\begin{bmatrix} \alpha_3 & \alpha_2\\ \alpha_4 & \alpha_1\end{bmatrix} \tag{104}$$

exists and satisfies the relation

$$\mathrm{F}_{0\alpha}\begin{bmatrix} \alpha_2 & \alpha_1\\ \alpha_2 & \alpha_1\end{bmatrix}\mathrm{F}''_{\alpha 0}\begin{bmatrix} \alpha_2 & \alpha_2\\ \alpha_1 & \alpha_1\end{bmatrix} = \frac{B_0 B(\alpha)}{B(\alpha_2)B(\alpha_1)}, \tag{105}$$

where $B(\alpha) = \sin 2b(\alpha - \delta)\sin 2b^{-1}(\delta - \alpha)$. Equation (105) can be verified with the help of the explicit expressions for the objects involved.

The relation (105) is particularly suggestive in view of the fact that S_{0r} gets identified with the so-called quantum dimension in the correspondence between modular functors and modular tensor categories [2]. What appears on the right hand side of (105) is related to the measure $d\mu_{\mathrm{Pl}}$ via $d\mu_{\mathrm{Pl}}(\alpha) = d\alpha B(\alpha)$, with $d\alpha$ being the standard Lebesque measure on $\mathbb{T}$.

This measure can be seen as the most natural counterpart of the quantum dimension in the nonrational case. This is seen most clearly when considering the quantum group structure[10] associated to a rational modular functor [26]. The quantum dimension represents the weight of a representation in the Plancherel (or Peter-Weyl) decomposition of the space of functions on the quantum group. As mentioned above, there is a quantum group "dual" to the modular functor defined by the representation theory of the Virasoro algebra with $c > 25$ [28, 34]. The natural measure appearing in the decomposition of the space of functions on the corresponding quantum group is precisely $d\mu_{\mathrm{Pl}}$ [28].

It is clearly an important open task for the future to analyze more systematically the set of relations that can be obtained in such a way.

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[10] More precisely: weak Hopf algebra structure.

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Kinetically Constrained Models

Nicoletta Cancrini, Fabio Martinelli, Cyril Roberto and Cristina Toninelli

Abstract Kinetically constrained spin models (KCSM) are interacting particle systems which are intensively studied in physics literature as models for systems undergoing glass or jamming transitions. KCSM leave on discrete lattices and evolve via a Glauber-like dynamics which is reversible w.r.t. a simple product measure. The key feature is that the creation/destruction of a particle at a given site can occur only if the current configuration satisfies proper local constraints. Due to the fact that creation/destruction rates can be zero, the whole analysis of the long time behavior becomes quite delicate. From the mathematical point of view, the basic issues concerning positivity of the spectral gap inside the ergodicity region and its scaling with the particle density remained open for most KCSM (with the exception of the East model in $d = 1$ Aldous and P. Diaconis, J. Stat. Phys. 107(5–6):945–975 2002). Here we review a novel multi-scale approach which we have developed in Cancrini et al. (Probab. Theory Relat. Fields 140:459–504, 2008; Lecture Notes in Mathematics, vol. 1970, pp. 307–340, Springer, 2009) trough which we: (i) prove positivity of the spectral gap in the whole ergodic region for a wide class of KCSM on $\mathbb{Z}^d$, (ii) establish (sometimes optimal) bounds on the behavior of the spectral gap near the boundary of the ergodicity region and (iii) prove pure exponential decay at equilibrium for the persistence function, i.e. the probability that the occupation variable at the origin does not change before time t. Our findings disprove certain

Nicoletta Cancrini
Dip. Matematica, Univ. l'Aquila, 1-67100 L'Aquila, Italy, e-mail: nicoletta.cancrini@roma1.infn.it

Fabio Martinelli
Dip. Matematica, Univ. Roma Tre, Largo S.L. Murialdo, 00146, Rome, Italy, e-mail: martin@mat.uniroma3.it

Cyril Roberto
L.A.M.A., Univ. Marne-la-Vallée, 5 bd Descartes, 77454 Marne-la-Vallée, France, e-mail: cyril.roberto@univ-mlv.fr

Cristina Toninelli
LPMA and CNRS UMR 7599, Univ. Paris VI–VII, 4, Pl. Jussieu, 75252 Paris Cedex 05, France, e-mail: cristina.toninelli@upmc.fr

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conjectures which appeared in the physical literature on the basis of numerical simulations. In particular (i) above establishes exponential decay of auto-correlation functions disproving the stretched exponential decay which had been conjecture for some KCSM and (ii) disproves some of the scalings which had been extrapolated from numerical simulations for the relaxation times (inverse of the spectral gap).

Many fascinating questions still remain unsettled for condensed matter physicists who study the *glass* and *jamming transitions*. These phenomena, which lead to the formation of amorphous solids, occur in several microscopically different systems as supercooled liquids, colloidal suspensions and vibrated granular materials [9, 27]. Basic *glassy properties* include a dramatic slowing down of dynamics when a proper external parameter is tuned (e.g. temperature is lowered for liquids) and the occurrence of a complicated relaxation: non exponential and spatially heterogeneous. When relaxation times become longer than experimental scales, equilibrium can no more be achieved: the system undergoes a dynamical arrest and freezes into an amorphous phase (the glass). The main issues in understanding these phenomena remain unsolved. In particular, it is not clear whether the dynamical arrest is due to the proximity of a phase transition and whether this is a static or purely dynamical one. The experiments on molecular liquids show that, if such an *ideal glass transition* occurs, it should have an unconventional behavior with *mixed first and second order features*. On the one hand, the divergence of relaxation times and the fact that both entropy and internal energy seem continuous is indicative of a second order transition. On the other hand a discontinuous order parameter is detected: the height of the plateau of the Fourier transform of the density–density correlation has a finite jump. This corresponds to the fact that the modulation of the microscopic density profile of the glass does not appear continuously from the flat liquid profile. Besides these mixed first/second order properties, another unconventional feature concerns the scaling of relaxation times which increase much more rapidly than for conventional second order transitions. Indeed most liquids display a faster than power law divergence around the glass transition, a signal of a cooperative relaxation on increasingly large scales as the temperature is decreased towards the transition. A very successful fit is the Vogel-Fulcher law: $\log \tau \simeq 1/(T - T_0)$. Finally another puzzling features is the absence of any experimental evidence of a static diverging correlation length: typical glass configurations are not very different from instantaneous configurations of the liquid and the dramatic slowing down of dynamics is apparently not due to an increasing long range order. An enormous amount of theoretical approaches has been proposed in the last fifty years to describe these phenomena. Among the theories which assume that a thermodynamic glass transition takes place at a finite temperature we recall mode coupling theories [14] and the random first order scenario [20]. Here we deal instead with Kinetically Constrained Models (KCM) which have been introduced in the 80's (see [24] for a review) and are based on the ansatz of a purely dynamical transition. The latter

would be the result of the geometrical constraints on the rearrangements of molecules which become more and more important as the temperature of the liquid is lowered (the density is increased).

KCM are stochastic lattice gases with hard core exclusion, namely on each site there is one or zero particle. The configuration on a lattice Λ is thus defined by assigning to each $x \in \Lambda$ its occupation variable: $\eta_x = 1$ or $\eta_x = 0$ if the site is occupied or empty, respectively. The dynamics is given by a continuous time Markov process which consists of a sequence of jumps for models with conservative (Kawasaki) dynamics and creation/destruction of particles for models with non conservative (Glauber) dynamics. The former are also known as Kinetically Constrained Lattice Gases (KCLG) and the latter as Kinetically Constrained Spin Models (KCSM)[1] (the occupation variables can indeed be interpreted as up and down spins which can be flipped). For all the models introduced in physics literature dynamics satisfies detailed balance w.r.t. to Bernoulli product measure (see instead [6] for the extension to models which are reversible w.r.t. high temperature Gibbs measures). Thus there are no static interactions beyond hard core and an equilibrium transition cannot take place. The key feature of both KCSM and KCLG is that an elementary move can occur only if the configuration verifies proper local constraints besides hard core. The latter mimic the geometric constraints on the possible rearrangements in physical systems, which could be at the root of the dynamical arrest [13, 21]. As we shall discuss, numerical simulations show that for proper choices of the constraints KCM indeed display glassy features. These include heterogeneous relaxation, faster than power law divergence of relaxation times τ and dynamical transitions. Therefore several analytical and numerical works have recently attempted to understand the mechanism which induces these glassy properties and to derive the typical time/length scales which are involved. Numerical simulations are however very delicate due to the rapid divergence of τ as the particle density p is increased as well as the non-trivial scaling of finite size effects. (Note that in order to compare with the above discussion on liquid/glass transition one should perform the change $p \to 1/(1+\exp(-1/T))$ to have temperature rather than density as the control parameter.)

Here we review our recent mathematical results [8, 6, 7] on KCM which have contributed to settle some debated questions arising in numerical simulations. In particular in [8] we have introduced a new technique trough which we obtain upper and lower bounds on the spectral gap of the Markov process and therefore on the relaxation time τ which, as we shall see, is directly related to the inverse of the spectral gap. We focus for simplicity on KCSM and discuss only at the end the more recent results [7] for KCLG. The dynamics of a KCSM on an integer lattice $\Lambda \subset \mathbb{Z}^d$ is precisely defined as follows. Each site waits an independent mean one exponential time and then, provided that the current configuration satisfies a local constraint which does not involve η_x, it refreshes its state. This is set to occupied with probability p and empty with probability $q = 1 - p$. In other words, if $c_x(\eta)$

[1] In physics literature the equivalent terminology "Facilitated Spin Models" is also used which, instead of emphasizing the presence of constraints, puts the accent on the complementary fact that proper events facilitate, i.e. allow, the elementary moves.

is the function which equals one (zero) when the constraint is (is not) verified, each site changes its current state with rate $c_x(\eta)[(1-p)\eta_x + p(1-\eta_x)]$. Since $c_x(\eta)$ does not depend on η_x detailed balance w.r.t. Bernoulli(p) measure μ_p is easily verified and μ_p is an invariant measure. As a direct consequence of the fact that the rates can degenerate to zero, there exist blocked configurations (s.t. on each site the constraint is not satisfied) as well as configurations which are not blocked but nevertheless contain a frozen backbone, i.e. a subset of sites on which for sure the constraint is not verified at any instant of time. Thus μ_p is not the unique invariant measure, for example any measure concentrated on a blocked configuration is also invariant. By taking proper superpositions of blocked configurations it is also possible to construct stationary measures which are also translational invariant (see [22] for a more detailed discussion). In order to model the geometric constraints on highly dense liquids, c_x usually specifies the maximal number of occupied sites in a proper neighborhood of x. Thus the dynamics becomes increasingly slow as p is increased and an ergodicity breaking transition may occur at a finite critical density, $p_c < 1$. More precisely, if we denote by $\mathscr{L}$ the generator of the Markov process on $\mathbb{Z}^d$, p_c separates the density regime in which the semigroup $P_t := e^{t\mathscr{L}}$ does (does not) converge to μ_p in the large time limit, namely $\lim_{t\to\infty} P_t f = \mu_p(f)$ for all $f \in L^2(\mu_p)$ iff $p < p_c$. As it is explained in Sect. 2.3 of [8], the dynamical arrest at p_c corresponds to the fact that an infinite spanning cluster of mutually blocked particles occurs. One of the main issues studied in physics literature is the long-time dynamics in the ergodic regime, in particular the scaling of the typical times when p approaches p_c from below. The most studied dynamical quantities are the spin-spin time auto-correlation $C(t)$ and the persistence function $F(t)$ defined as follows

$$C(t) := \int d\mu_p(\eta(0))\eta_0(0)E_\eta[\eta_0(t)] - p^2$$

where $E_{\eta(0)}[f(\eta(t))]$ is the expectation over the Markov process at time t when the initial configuration is $\eta(0)$ and

$$F(t) := \int d\mu_p(\eta(0))P[\eta_0(s) = \eta_0(0)\ \forall s < t],$$

namely $F(t)$ is the probability that up to time t the occupation variable of the origin has never changed. A first key issue is whether $C(t)$ and $F(t)$ decay exponentially as for the unconstrained models (i.e. for $c_x(\eta) = 1$). Furthermore one would like to determine the scalings with p of the typical time scale τ which enter in their decay. By analyzing the spectral gap of the generator $\mathscr{L}$, namely

$$\mathrm{gap}(\mathscr{L}) := \inf_{\substack{f\in L^2(\mu_p)\\ f\neq const.}} \frac{\mu_p(f, -\mathscr{L}f)}{\mu_p(f-\mu_p(f))^2} \tag{1}$$

and using the Poincaré inequality

$$\mathrm{Var}(P_t(f)) \le \exp(-2t\ \mathrm{gap}(\mathscr{L}))\mathrm{Var}(f) \tag{2}$$

and the inequality established in Theorem 3.6 of [8] via a Feynman-Kac bound

$$F(t) \leq \exp(-qtc\text{gap}) \tag{3}$$

where c is a constant independent on q, we will obtain rigorous answers to the above questions. In particular a strictly positive spectral gap together with (2) and (3) imply an exponential decay for both $C(t)$ and $F(t)$. As we will detail below, in some cases we prove and in other cases we disprove the conjectures in physics literature. Note that the above Poincaré inequality means that the inverse of the spectral gap is the worst relaxation time over all one time quantities. Thus, when referring to our results, τ will always stand for $1/\text{gap}$. Analogously $\tau(L)$ will be the inverse of the spectral gap of the generator of the process restricted to a square lattice Λ_L of linear size L (with properly specified boundary conditions).

Let us recall a standard classification before introducing the specific choices of the constraints that we analyze. KCSMs can be divided into two classes: (i) non-cooperative and (ii) cooperative models. For the former it is (for the latter it is not) possible to construct an allowed path which completely empties *any* configuration which contains somewhere a proper finite cluster of vacancies. Non-cooperative models are ergodic at any density, namely $p_c = 1$, while p_c is finite for some of the cooperative models. Thus we can further classify cooperative models into: (iia) models that are ergodic in the thermodynamic limit at any $p < 1$, i.e. $p_c = 1$; (iib) models that display an ergodicity breaking transition at $p_c < 1$. Cooperative models are usually considered more interesting since their relaxation involves the collective rearrangements of increasingly large regions as the density increases, analogously to what experiments suggest near the glass transition.

Among non cooperative models we recall the Fredrickson-Andersen [13] one spin facilitated (FA1f) for which a move at x is allowed only if at least one of its nearest neighbors is empty: $c_x(\eta) = 1$ if $\sum_{y\ n.n.x}(1-\eta_x) > 0$, $c_x(\eta) = 0$ otherwise. In this case the presence of a single vacancy allows to empty the whole lattice. In [3, 4] a dynamical field theory was derived yielding an exponential decay for $C(t)$ with a typical scale for $q \to 0$ as $\tau \propto 1/q^z$ with $z = 3$ for $d = 1$, $z = 2 + \epsilon(d)$ with $\epsilon(2) \simeq 0.3$, $\epsilon(3) \simeq 0.1$ and $\epsilon(d \geq 4) = 0$. An exact mapping into a diffusion limited aggregation model and its renormalization [18] gives instead $d = 2$ as the upper critical dimension and $\epsilon(d) = 0$ in $d \geq 2$. Our results are: gap $\propto q^3$ in $d = 1$, $q^2/|\log q| \leq \text{gap} \leq q^2$ in $d = 2$ and $q^2 \leq \text{gap} \leq q^{1+2/d}$ in $d = 3$. Thus we get $\epsilon(2) = 0$ and $\epsilon(3) \leq 0$, disproving the findings in [3, 4] and confirming those in [18].

Another popular model is the one-dimensional East model [10] for which the constraint requires a vacancy on the right nearest neighbor, i.e. $c_x(\eta) = (1 - \eta_{x+1})$. On a finite volume the presence of a single vacancy on the rightmost site allows to empty the whole lattice. However the East does not belong to the non-cooperative class since, due to the directed nature of constraints, the vacancy should occur in a specific position and the relaxation involves the cooperative rearrangements of large regions as $p \to 1$. The scaling $\log \tau \sim (\log(1/q))^2$ had indeed been conjectured in [10, 11] and proved in [2]. In [8] we prove the exact asymptotics

$\log \tau = c(\log(1/q))^2$ where $c = 1/(2\log 2)$. Our result differs from the $c = 1/\log 2$ value incorrectly derived in [11]. As we clarify in [6], this is due to the fact that the relation between length and time scales extrapolated in [11] from coarsening dynamics does not lead to the correct equilibrium result unless relaxation on scales smaller than the typical distance of two vacancies is also taken into account.

Among cooperative models without transition (iia) we consider instead FAjf on an hyper-cubic lattice of dimension d with $2 \le j \le d$ [13]: the constraint requires at least j empty nearest neighbours. As can be directly checked, for all these models it is not possible to devise a finite seed of vacancies which allows emptying the whole lattice, thus the models are cooperative. Consider, e.g., the case $d = 2$, $j = 2$ (with periodic boundary conditions) and focus on a configuration which contains two adjacent rows which are completely filled. It is easy to verify that these particles can never be erased, not even if the rest of the lattice is completely empty. The upper restriction on j comes from the fact if $j > d$ there exist finite sets of forever blocked particles. Thus a fraction of the system is frozen at all densities ($p_c = 0$) and the models are not suitable to describe the slow dynamics close to glass-jamming transitions. The choices which have been most studied in physics literature are $j = 2$ both in $d = 2$ and $d = 3$ and $j = 3$ in $d = 3$. In all cases stretched exponential relaxation has been numerically detected: $C(t)$ and $F(t)$ are fitted with $\exp(-(t/\tau)^\beta)$ with β decreasing as the density p is increased [15, 12, 16]. For the scaling of τ with p, as pointed out in [24], little is known beyond the general recognition that the behavior is reminiscent to the one of supercooled liquids. Among the different forms proposed for FA2f we recall Vogel-Fulcher [15] and $\exp(c/q)$ [5]. The latter form is supported by the conjecture that relaxation occurs via the diffusion of critical droplets of size $1/q$ over distances $\exp(c/q)$ [23]. Our results are as follows. For all $j \le d$ and all dimensions we prove that the spectral gap is strictly positive for $p < p_c = 1$: exponential relaxation occurs both for $C(t)$ and $F(t)$ contradicting the stretched exponential conjecture of [15, 16, 12] and confirming the exponential decay derived in [11]. Furthermore for FA2f and FA3f we prove $\exp q^{-1} \le \tau \le \exp q^{-5}$ and $\exp\exp q^{-1} \le \tau \le \exp\exp q^{-2}$, respectively. Thus we establish a super-Arrhenius scaling compatible with [5, 23] and exclude the form proposed in [15]. Also, we believe that the upper bound for FA2f can be ameliorated to $\tau \le \exp q^{-2}$.

Among (iib) models, we consider the two dimensional North-East and the Spiral models. For the former [19] both the up ($x + \mathbf{e}_2$) and right ($x + \mathbf{e}_1$) neighbors should be empty in order for a move at x to be allowed ($\mathbf{e}_i$ are the unit basis vectors). For the Spiral model [25] the constraint is more complicated. Let the NE, NW, SW and SE neighbours of x be defined respectively as $(x + \mathbf{e}_2, x + \mathbf{e}_1 + \mathbf{e}_2)$, $(x - \mathbf{e}_1, x - \mathbf{e}_1 + \mathbf{e}_2)$, $(x - \mathbf{e}_2, x - \mathbf{e}_1 - \mathbf{e}_2)$ and $(x + \mathbf{e}_1, x + \mathbf{e}_1 - \mathbf{e}_2)$. Then the constraint at x goes as follows: (a) the two NE and/or the two SW neighbours of x should be empty and (b) the two NW and/or the two SE neighbours of x should be empty too. For both the North-East and Spiral model the cluster of frozen particles arises at $p_c = \rho_{dp}$ with ρ_{dp} the critical density of directed percolation. In the case of North-East there is a trivial one to one correspondence between directed percolation clusters and frozen clusters. As a consequence the transition is continuous, namely

the density of the frozen backbone is zero at p_c. Instead for the Spiral model the mechanism is much more subtle [25]: the presence of proper directed clusters imply the occurrence of blocked clusters but the converse is not true. Indeed the proof of $p_c = \rho_{dp}$ is much more involved [25] and the transition is here due to the interaction between two independent directed percolation processes. Furthermore the transition is expected to display mixed first/second order features [25, 26]: the density of the frozen backbone is finite at p_c and the size of the frozen cluster diverges as $p \nearrow p_c$. Thus the Spiral model is a KCSM whose ergodicity breaking transition has the features of an ideal glass transition. For both North-East and Spiral models we prove that the spectral gap in infinite volume is strictly positive for any $p < p_c$. Therefore in the whole ergodic region $C(t)$ and $F(t)$ decay exponentially. At criticality, $p = \rho_{dp}$, we prove that relaxation is instead polynomial or slower than polynomial in time. Finally, for $p > \rho_{dp}$, we prove that a strong signature of the infinite volume ergodicity breaking occurs if one considers the model on a finite volume of linear size L. The relaxation time is uniform on L for $p < p_c$ and diverges as $\tau(L) \propto \exp(L\, c(p))$ for $p > p_c$.

We will sketch our technique to derive the positivity of the spectral gap and its scaling when $p \nearrow p_c$ by focusing on FA2f in $d = 2$ (see [8] for rigorous proofs). We will comment at the end on the flexibility of the tools which allow indeed to deal with all the other choices of the constraints discussed above as well as with more general models, including those with long range constraints [7] and with static interactions other than hard core [6]. Before entering in the details we wish to underline that from the mathematical point of view the main difficulties come from the existence of several invariant measures and from the fact that KCSM are not attractive, thus the usual coupling arguments cannot be applied. Both features are a direct consequence of the constraints, i.e. of the fact that the creation/destruction rates may degenerate to zero. This explains why the basic issues concerning the large time behavior of KCSM are non trivial and why they remained open for most of the interesting models, with the notable exception of the East for which in [2] the positivity of the spectral gap had been established. However the method of [2] uses the specifics of the East model and it cannot be applied neither to higher dimensions nor to the above discussed cooperative models which are relevant for physics literature.

In order to study the spectral gap of FA2f we proceed as follows. First we introduce an auxiliary KCSM model, the *General Model* (*GM*), which has N-valued occupation variables and we study its relaxation time, τ_{GM}. Then we establish an upper bound on the relaxation time for FA2f, τ_{FA}, by using a renormalization procedure which forces the GM constraints on scales larger than a proper block size and leaves inside each block the original FA2f dynamics. Finally we derive a lower bound on τ_{FA} by using the knowledge of the typical regions which have to be rearranged to create/destruct a particle.

Let $n_x \in S$ be an N-valued occupation variable and choose a probability measure, ν, on S. We identify a subset G of S which we call the *good event* and we say that a site x is *good* if $n_x \in G$. GM dynamics is defined as follows. Each site x waits a mean one exponential time and then n_x is refreshed by a new

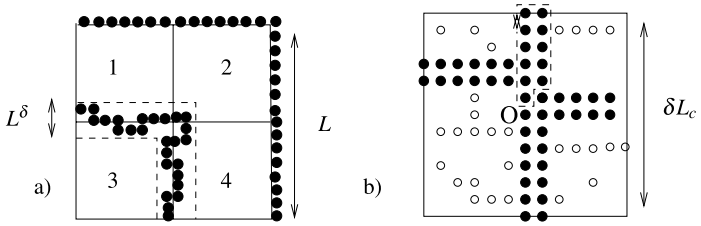

Fig. 1 (a) Block dynamics for GM: percolating path of good sites (•) required to renew configuration on 3. (b) Blocking event for FA2f. • (○) stand for particles which do (do not) belong to the backbone. Sites inside dotted line form one of the sequences of $\geq \delta L_c/2$ sites to be emptied before O

value n'_x sampled from ν, provided its North, North-East and East neighbors (i.e. $x + \mathbf{e}_1, x + \mathbf{e}_1 + \mathbf{e}_2, x + \mathbf{e}_2$) are good. If this constraint is not satisfied n_x remains unchanged. We consider GM on a square lattice Λ_L of linear size L with good boundary conditions on the top and right boundaries to ensure ergodicity (i.e. the existence of an allowed path which connects any two configurations which in finite volume guarantees $\tau_{GM}(L) < \infty$). In order to evaluate $\tau_{GM}(L)$ we follow a *bisection-constrained method*. Partition Λ_L into four blocks as in Fig. 1a) and define the following auxiliary block accelerated dynamics. Each block waits a mean one exponential time and then its configuration is replaced by a new one chosen according to the product equilibrium probability given by ν. On the top right block (block 2 in Fig. 1a)) this move is always allowed. For the others, a constraint should be satisfied: on an l-shaped frame of width L^δ, $\delta < 1$, there should be a percolating cluster of good sites as in Fig. 1a). In other words the constraint requires the good GM boundary conditions on block 3 (see Fig. 1a)) and the same for blocks 1 and 4 (instead on block 2 they are automatically guaranteed by the boundary condition on Λ_L). Then

$$\tau_{GM}(L) \leq \tau^{GM}_{\text{block}}(L)\tau_{GM}(L/2)$$

with $\tau^{GM}_{\text{block}}(L)$ the relaxation time for the block dynamics. The above inequality (see [8] for a rigorous proof) corresponds intuitively to a two step relaxation: first on the block scale, then inside each individual block. If the probability that a site is good, $\nu(G)$, is larger than the threshold of site percolation ρ_{sp} the constraint of the block dynamics is satisfied with probability $\sim 1 - \exp(-mL^\delta)$ and $\tau^{GM}_{\text{block}}(L) \simeq (1 + \exp(-mL^\delta))$. Then, by dividing $\Lambda_{L/2}$ into four blocks and so on up to constant size, we get

$$\tau_{GM}(L) \leq c \prod_n \tau^{GM}_{\text{block}}(2^{-n}L),$$

where c is a finite constant and the product contains $O(\log L)$ terms. Therefore we get a bound for $\tau_{GM}(L)$ which does not dependent on L provided the product over the τ^{GM}_{block}'s converges. From the above observation, this certainly occurs for $\nu(G) > \rho_{sp}$.

Let us now consider FA2f in $d = 2$ on Λ_L with empty boundary conditions on the top and right borders. We partition Λ_L into disjoint blocks of size $k\,L_c$, where $k \gg 1$ and $L_c = \exp(\pi^2/(18q))$. We can now define the following auxiliary dynamics: each block waits a mean one exponential time and then its configuration is replaced by a new one chosen according to μ_p provided the three neighbouring blocks in the North, East and North-East direction are *internally spanned*. By internally spanned we mean that each of these blocks can be completely emptied by a proper sequence of allowed moves when we consider occupied boundary conditions on it. The probability that a block of linear size ℓ is internally spanned has been evaluated in the context of bootstrap percolation: it goes to one exponentially fast when ℓ exceeds the crossover length L_c defined above [1, 17]. Applying as before a two step relaxation argument, we get $\tau_{FA}(L) \le \tau^{FA}_{\text{block}}(L)\,\tau_{FA}(kL_c)$ where $\tau^{FA}_{\text{block}}(L)$ is the relaxation time of the above defined block dynamics, which a priori depends on the number of blocks and therefore on L. We will now show that $\tau^{FA}_{\text{block}}(L) \simeq 1$. Take a square lattice with $(L/kL_c)^2$ sites and define on each site a $2^{(kL_c)^2}$-valued occupation variable, n_x, belonging to $S = (0, 1)^{(kL_c)^2}$. It is immediate to verify that S and $S^{(L/kL_c)^2}$ are the configuration space of FA2f on a block of size kL_c and on Λ_L, respectively. Furthermore, in terms of the n_x variables, the above defined block dynamics coincides with GM with the choices: n_x is good when the corresponding block in Λ_L is internally spanned and ν equals μ_p restricted to the block. Therefore, thanks to this mapping and our result for τ_{GM}, we get $\tau^{FA}_{\text{block}}(L) = \tau^{GM}(L/kL_c) \simeq 1$ since the probability of the good event "a block of size kL_c with $k \gg 1$ is internally spanned" is $\nu(G) \simeq 1$ [17]. A few remarks are in order. In our renormalization procedure we have forced on the block scale the directed GM constraint which is more restrictive than the one of FA2f. This choice, which is due to the necessity of boundary conditions which ensure ergodicity for FA2f dynamics inside each block [8], is allowed because we are deriving an upper bound on τ_{FA} and the effect of a stronger constraint is to slow down the dynamics. Furthermore, as explained above, for our choice of the block scale $\tau_{GM} \simeq 1$. This means that using GM instead of FA2f constraints on large blocks does not change the leading behavior of the upper bound. Putting above results together we conclude that $\tau_{FA}(L) \le \tau_{FA}(kL_c)$ and, since L_c depends on p but not on L and $L_c(p) < \infty$ for $p < p_c = 1$, the relaxation time of FA2f is uniformly bounded in L. This leads for any $p < 1$ to an exponential relaxation in the infinite volume limit for all one time functions as well as for the persistence function [8]. At the same time the density dependence of τ_{FA} is completely encoded in the size $L_c(p)$. To evaluate the latter we reduce the scale from L_c to $1/q^2$ via a strategy similar to the previous one. However, since on scales smaller than L_c the event "the block is internally spanned" becomes very unlikely, we are forced to make a different choice for the good event of the renormalized dynamics in order to keep $\tau_{\text{GM}} \simeq 1$. The new choice is suggested by the following two observations: (i) any straight empty segment of length ℓ can be displaced by one step in a given direction if there is at least one vacancy on the adjacent segment in that direction; (ii) the probability that there exists at least one vacancy on each segment of length ℓ inside a square of size L_c is very near to one as soon as

$\ell \gg 1/q^2$. Thus, we choose good events which force on Λ_{kL_c} at least one straight empty segment of length $1/q^2$ and at least one vacancy on all other segments of this length. By applying again a bisection procedure together with the construction of suitable paths which allow the creation/destruction of a particle starting from straight empty segment, we get $\tau_{FA}(L_c) \le cL_c\tau_{FA}(1/q^2)$ where the term L_c comes from the length of the path. Finally we bound $\tau_{FA}(1/q^2)$ with the highest entropy cost and get $\tau_{FA}(L) < cL_c \exp(1/q^2) = O(\exp(1/q^2))$.

In order to establish lower bounds for τ one can devise as usual a suitable choice of test functions and use the variational characterization of the spectral gap (1). In some cases it is however simpler to follow a strategy which uses the knowledge of the typical blocked configurations together with our bound for the persistence (3). Consider a set of configurations B, called the *blocking event*, and let $P_B(t)$ be the infimum over the initial configurations $\eta(0) \in B$ of the probability that the origin is occupied up to time t. The inequality (3) implies $\mu_p(B)P_B(t) \le \exp(-tq/\tau)$. For FA2f we define the blocking event B as the set of configurations for which, after standard bootstrap percolation inside $\Lambda_{\delta L_c}$ (i.e. after removing all particles which can be removed until exhausting the set of possible movements), a backbone of particles containing the origin survives. By choosing $\delta \ll 1$ and recalling the bootstrap percolation results of [1, 17] we have $\mu_p(B) \simeq 1$. In finite volume this backbone will eventually get unblocked thanks to the vacancies outside $\Lambda_{\delta L_c}$. However, this requires an ordered sequence of at least $\delta L_c/2$ moves (Fig. 1b). Thus, $P_B(t = \epsilon\delta L_c) \simeq 1$ for sufficiently small ϵ. Therefore $O(1) \le \exp(-tq/\tau)$ for $t \simeq \epsilon\delta L_c$, i.e. $\tau \ge O(L_c)$.

In conclusion we have developed a technique which allows to obtain rigorous results on τ_{FA} via the knowledge of the typical region which has to be emptied around a given site in order to perform a move on it. This size can in turn be determined via a deterministic procedure which corresponds to subsequently erase all particles which are unconstrained. The latter, due to the peculiar form of FA constraints, coincides with the very much studied bootstrap algorithm. Our main new results are exponential relaxation in the whole ergodic regime as well as faster than power law divergence of τ in $p - p_c$ when $p \nearrow p_c = 1$.

In higher dimensions and for the other KCSM one can proceed analogously [8]. The only delicate point is to choose an "internally spanned event" adapted to the constraints at hand, see e.g. [8] and [6] for the natural choices in the case of the North-East and the Spiral model, respectively. In some cases, e.g. for the Spiral model [6], even the form of the blocks for the partition of Λ_L before the renormalization procedure has to be adapted to the constraints leading to a non rectangular geometry. The scaling of τ on p depends on the specific choice of the constraints but in all cases the upper bound $\tau < \tau(L_c)$ holds, where L_c is the typical size over which the proper "internally spanned event" is likely to occur. The latter can be always determined via a properly modified bootstrap-like deterministic procedure [8] and it is finite for $p < p_c$. Thus we establish that the inverse of the spectral gap is finite which implies exponential relaxation for all one times quantities (e.g. $C(t)$) as well as for $F(t)$.

Furthermore proper modifications of the bisection-constrained technique also allow to deal with models which are reversible w.r.t. a high temperature Gibbs measure instead of μ_p [6] as well as models with long range constraints [7]. In both cases we establish positivity of the spectral gap in the whole ergodic region. The result for the long range models is particularly relevant since it allows, via proper renormalization and path techniques [7], to study the models with Kawasaki dynamics, namely the KCLG. In particular, by using the positivity of the spectral gap for a proper long range KCSM, we recently established [7] polynomial decay to equilibrium in infinite volume as well as $1/L^2$ decay for the spectral gap on finite volume with boundary sources for the most popular KCLG, the so called Kob-Andersen model [21].

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The Distributions of Random Matrix Theory and their Applications *

Craig A. Tracy and Harold Widom

Abstract This paper surveys the largest eigenvalue distributions appearing in random matrix theory and their application to multivariate statistical analysis.

1 Random Matrix Models: Gaussian Ensembles

A random matrix model (RMM) is a probability space $(\Omega, \mathbb{P}, \mathscr{F})$ where the sample space Ω is a set of matrices. There are three classic finite-N RMM called the *Gaussian ensembles* (see, e.g. [23] and for early history [30]):

- Gaussian Orthogonal Ensemble (GOE, $\beta = 1$)
  - $\Omega = N \times N$ real symmetric matrices
  - $\mathbb{P}$ = unique (up to a choice of the mean and variance) measure that is invariant under orthogonal transformations and the algebraically independent matrix elements are i.i.d. random variables. Explicitly (for mean zero and a choice of the variance), the density is

$$c_N \exp\bigl(-\operatorname{tr}(A^2)/2\bigr)\, dA, \tag{1}$$

    where c_N is a normalization constant and $dA = \prod_i dA_{ii} \prod_{i<j} dA_{ij}$, the product Lebesgue measure on the algebraically independent matrix elements.
- Gaussian Unitary Ensemble (GUE, $\beta = 2$)

Craig A. Tracy
Department of Mathematics, University of California, Davis, CA 95616, USA, e-mail: tracy@math.ucdavis.edu

Harold Widom
Department of Mathematics, University of California, Santa Cruz, CA 95064, USA, e-mail: widom@ucsc.edu

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- $\Omega = N \times N$ hermitian matrices
- $\mathbb{P}$ = unique measure (again up to a choice of the mean and variance) that is invariant under unitary transformations and the algebraically independent real and imaginary matrix elements are i.i.d. random variables. Again the density is of the form (1) with $dA = \prod_i dA_{ii} \prod_{i<j} d\,\mathrm{Re}(A_{ij})\, d\,\mathrm{Im}(A_{ij})$.

• Gaussian Symplectic Ensemble (GSE, $\beta = 4$) (see [23] for a definition)

For A in any of the above Gaussian ensembles, let $\lambda_1(A) \le \cdots \le \lambda_N(A) := \lambda_{\max}$ denote the eigenvalues of A. These eigenvalues are real and define random variables on the respective probability spaces. (With probability one the eigenvalues are distinct.) Since these Gaussian ensembles are defined by invariant measures, one can explicitly compute the joint distribution of eigenvalues and show that it has the following density with respect to Lebesgue measure:

$$\mathbb{P}_{\beta,N}(x_1, \ldots, x_N) = C_{N,\beta} \prod_{1\le i<j\le N} |x_i - x_j|^\beta \prod_{i=1}^{N} e^{-\beta x_i^2/2}, \quad \beta = 1, 2, 4,$$

where $C_{N,\beta}$ is a known normalization constant [23]. The form of the joint density explains the usefulness of the β notation.

1.1 Largest Eigenvalue Distributions F_β. Painlevé II Representations

Generally speaking, the interest lies in limit laws as $N \to \infty$. As is familiar from the central limit theorem, to get nontrivial limits one must center and normalize the random variables. Here the main focus is on the limit law associated with the largest eigenvalue. If

$$F_{N,\beta}(t) := \mathbb{P}_{\beta,N}\left(\lambda_{\max} < t\right), \quad \beta = 1, 2, 4,$$

denotes the distribution function of the largest eigenvalue, then the basic limit laws [37–39] state that[1]

$$F_\beta(x) := \lim_{N\to\infty} F_{N,\beta}\left(2\sigma\sqrt{N} + \frac{\sigma x}{N^{1/6}}\right), \quad \beta = 1, 2, 4,$$

exist and are given explicitly by

$$F_2(x) = \exp\left(-\int_x^\infty (y - x)q^2(y)\, dy\right) \tag{2}$$

[1] Here σ is the standard deviation of the Gaussian distribution on the off-diagonal matrix elements. For the normalization we've chosen, $\sigma = 1/\sqrt{2}$; however, other choices are common.

where q is the unique solution[2] to the *Painlevé II equation*

$$\frac{d^2q}{dx^2} = xq + 2q^3$$

satisfying the boundary condition[3]

$$q(x) \sim \mathrm{Ai}(x) \quad \text{as } x \to \infty. \tag{3}$$

It is known [17] that

$$q(x) = \sqrt{-\frac{x}{2}}\left(1 + \frac{1}{8x^3} + \mathrm{O}\left(\frac{1}{x^6}\right)\right) \quad \text{as } x \to -\infty.$$

The orthogonal and symplectic distributions [39] are

$$F_1(x) = \exp\left(-\frac{1}{2}\int_x^\infty q(y)\,dy\right)(F_2(x))^{1/2}, \tag{4}$$

$$F_4(x/\sqrt{2}) = \cosh\left(\frac{1}{2}\int_x^\infty q(y)\,dy\right)(F_2(x))^{1/2}. \tag{5}$$

Graphs of the densities $f_\beta := dF_\beta/dx$ are in Fig. 1 and some statistics of F_β can be found in the Table 1.

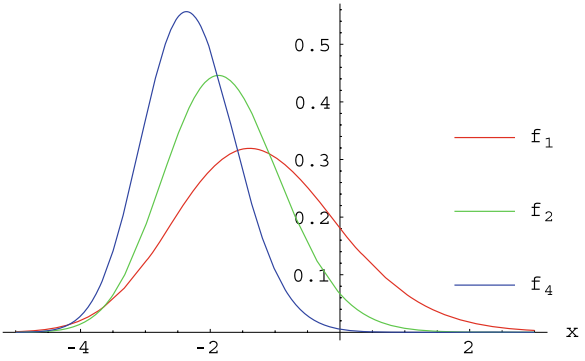

Fig. 1 Largest eigenvalue densities $f_\beta(x) = dF_\beta/dx$, $\beta = 1, 2, 4$ where F_β are defined in (2), (4) and (5)

[2] That such a unique solution exists is a nontrivial fact first proved by Hastings and McLeod [17]; and for this reason, q is often called the Hastings-McLeod solution. See [15] for a detailed account of Painlevé transcendents.

[3] Ai is the Airy function.

1.1.1 Tail behavior of F_β

The asymptotics for $F_\beta(x)$ as $x \to +\infty$ follows straightforwardly from (2)–(5). To state the results it is first convenient to introduce

$$F(x) = \exp\left(-\frac{1}{2}\int_x^\infty (y-x)q(y)^2\,dy\right),$$
$$E(x) = \exp\left(-\frac{1}{2}\int_x^\infty q(y)\,dy\right)$$

so that

$$F_1(x) = E(x)F(x), \qquad F_2(x) = F(x)^2, \quad \text{and}$$
$$F_4(x/\sqrt{2}) = \frac{1}{2}\left(E(x) + \frac{1}{E(x)}\right)F(x).$$

Then as $x \to +\infty$

$$F(x) = 1 - \frac{e^{-\frac{4}{3}x^{3/2}}}{32\pi x^{3/2}}\left(1 + \mathrm{O}\left(\frac{1}{x^{3/2}}\right)\right),$$
$$E(x) = 1 - \frac{e^{-\frac{2}{3}x^{3/2}}}{4\sqrt{\pi}x^{3/2}}\left(1 + \mathrm{O}\left(\frac{1}{x^{3/2}}\right)\right)$$

from which the asymptotics for F_β follows.

The asymptotics as $x \to -\infty$ are much more difficult and the complete solution was only recently achieved for $\beta = 1, 2, 4$ [4]. We quote the final results and refer the reader to [4] for a history of this problem. As $x \to -\infty$

$$F_1(x) = \tau_1 \frac{e^{-\frac{1}{24}|x|^3 - \frac{1}{3\sqrt{2}}|x|^{3/2}}}{|x|^{1/16}}\left(1 - \frac{1}{24\sqrt{2}|x|^{3/2}} + \mathrm{O}\left(|x|^{-3}\right)\right),$$
$$F_2(x) = \tau_2 \frac{e^{-\frac{1}{12}|x|^3}}{|x|^{1/8}}\left(1 + \frac{3}{2^6|x|^3} + \mathrm{O}\left(|x|^{-6}\right)\right),$$
$$F_4(x/\sqrt{2}) = \tau_4 \frac{e^{-\frac{1}{24}|x|^3 + \frac{1}{3\sqrt{2}}|x|^{3/2}}}{|x|^{1/16}}\left(1 + \frac{1}{24\sqrt{2}|x|^{3/2}} + \mathrm{O}\left(|x|^{-3}\right)\right)$$

where

$$\tau_1 = 2^{-11/48}e^{\frac{1}{2}\zeta'(-1)}, \qquad \tau_2 = 2^{1/24}e^{\zeta'(-1)}, \qquad \tau_4 = 2^{-35/48}e^{\frac{1}{2}\zeta'(-1)}$$

and $\zeta'(-1) = -0.1654211437\ldots$ is the derivative of the Riemann zeta function evaluated at -1.

1.1.2 Numerical evaluation of F_β

Particularly for applications to data analysis, it is useful to have numerical evaluations of the distributions F_β. Chapter 7 of Dieng's Ph.D. thesis [12] gives MATLAB^{TM} code to evaluate and plot these distributions. Tables of the Hastings-McLeod solution to Painlevé II and $F_{1,2}$ can be found on Prähofer's homepage [31].[4] A different approach [6] to the numerical evaluation of F_β is based on the Fredholm determinant representations for F_β (see, e.g. [40]).

Table 1 The mean (μ_β), variance (σ_β^2), skewness (S_β) and kurtosis (K_β) of F_β. The high-precision numbers are courtesy of Michael Prähofer and Folkmar Bornemann

β	μ_β	σ_β^2	S_β	K_β
1	−1.206 533 574	1.607 781 034	0.293 464 524	0.165 242 938
2	−1.771 086 807	0.813 194 792	0.224 084 203	0.093 448 087
4	−2.306 884 893	0.517 723 721	0.165 509 494	0.049 195 157

1.2 Next-Largest, Next-Next Largest, Etc. Eigenvalue Distributions

There exist Painlevé II type representations for the limiting distributions of the next-largest eigenvalue (λ_{N-1}), next-next largest eigenvalue (λ_{N-2}), etc. The unitary case was examined some time ago [38] but only recently did Dieng [11] derive limiting distributions for the orthogonal and symplectic cases. It should be remarked that the results in the orthogonal case were somewhat surprising. Figure 2 displays simulations for the four largest eigenvalues of $N = 1000$ GOE matrices and their respective limiting distributions.

2 Universality Theorems

A natural question is to what extent do the above limit laws depend upon the Gaussian and invariance assumptions for the probability measure?

2.1 Invariant Ensembles

A more general class of invariant RMM results by replacing the Gaussian measures with

[4] Note that the Hastings-McLeod solution in the Prähofer tables is denoted $u(s)$ and in the notation here $u(s) = -q(s)$.

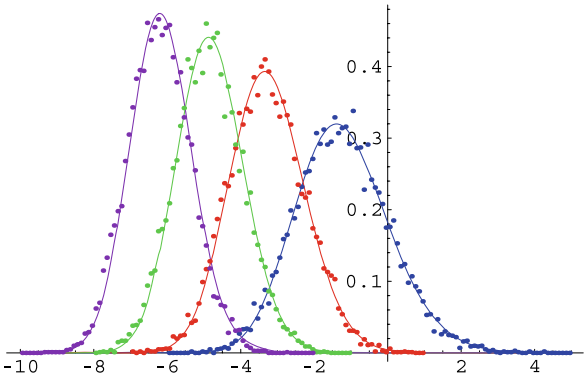

Fig. 2 A histogram of the four largest (centered and normalized) eigenvalues for 10^4 realizations of $10^3 \times 10^3$ GOE matrices. Solid curves are the limiting distributions from [11]. Figure a courtesy of Momar Dieng

$$d\mathbb{P}_N(A) = c_{N,\beta} \exp\left(-\beta \operatorname{tr}(V(A))/2\right) dA$$

where V is a polynomial of even degree and positive leading coefficient. This implies that the joint density for the eigenvalues is

$$\mathbb{P}_{\beta,V,N}(x_1, \ldots, x_N) = C_{V,N,\beta} \prod_{1 \le i < j \le N} |x_i - x_j|^\beta \prod_{i=1}^{N} e^{-\beta V(x_i)/2}, \quad \beta = 1, 2, 4, \tag{6}$$

where $C_{V,N,\beta}$ is a normalization constant [23]. Unitary ensembles ($\beta = 2$) are technically simpler than the orthogonal and symplectic ensembles ($\beta = 1, 4$), but both require for general V powerful Riemann-Hilbert methods [9] for the asymptotic analysis. The main conclusions from these studies for the limiting distribution of the largest eigenvalue are

Theorem 1. *There exist constants $z_N^{(\beta)}$ and $s_N^{(\beta)}$ such that*

$$\lim_{N\to\infty} \mathbb{P}_{\beta,V,N}\left(\frac{\lambda_{\max} - z_N^{(\beta)}}{s_N^{(\beta)}} \le t\right) = F_\beta(t), \quad \beta = 1, 2, 4,$$

where the F_β are given by (2), (4) *and* (5).

The results for the unitary case ($\beta = 2$) are due to Deift, Kriecherbaur, McLaughlin, Venakides and Zhou [10] and the orthogonal/symplectic results are recent work of Deift and Gioev [8]. The universality theorem for special case $V(A) = \frac{1}{4}A^4 - gA^2$ is due to Bleher and Its [5] ($\beta = 2$) and Stojanovic [36] ($\beta = 1$). These deep theorems broadly extend the domain of attraction of the F_β limit laws. Deift's ICM 2006 lecture [7] is a recommended overview for these developments.

2.2 Wigner Ensembles

Wigner matrices are RMM of complex hermitian or real symmetric $N \times N$ matrices H

$$H = \frac{1}{\sqrt{N}}(A_{ij})_{i,j=1}^{N}$$

where A_{ij}, $1 \leq i < j \leq N$ are i.i.d. complex or real random variables with distribution μ. The diagonal matrix elements are i.i.d. real random variables independent of the off-diagonal elements. The diagonal probability distribution is centered, independent of N and has finite variance. They are called *Wigner matrices* since Wigner in 1955 first studied the limiting distribution of the empirical spectral measure under the assumption that μ has finite variance. The limiting spectral measure is the famous *Wigner semicircle* distribution. We denote the Wigner measure on the space of either complex Hermitian or real symmetric $N \times N$ matrices by $\mathbb{P}_{W,N}$

Except in the case of the Gaussian distribution, the Wigner ensembles define non-invariant measures. For this reason no explicit formulas for the joint distribution of eigenvalues, such as (6) for invariant measures, are known. Thus the techniques used to prove universality theorems have a completely different flavor.

Soshnikov [33] proved, under the additional assumptions that μ is symmetric (all odd moments are zero) and the distribution decays as at least as fast as a Gaussian distribution together with a normalization on the variances,[5] the following universality statement for the largest eigenvalue $\lambda_{\max}$ of Wigner random matrices

Theorem 2.

$$\lim_{N\to\infty} \mathbb{P}_{W,N}\left(\lambda_{\max} \leq 1 + \frac{x}{2N^{2/3}}\right) = F_\beta(x)$$

with $\beta = 1$ for real symmetric matrices and $\beta = 2$ for complex hermitian matrices.

The importance of Soshnikov's theorem is the universality of F_β has been established for ensembles for which the "integrable" techniques, e.g. Fredholm theory, Riemann-Hilbert methods, Painlevé theory, are not directly applicable. Current research [29] is exploring the relaxation of the symmetry constraint on the underlying distribution μ.

3 Multivariate Statistical Analysis

As Johnstone [22] remarked:

> It is a striking feature of the classical theory of multivariate statistical analysis that most of the standard techniques—principal components, canonical correlations, multivariate analysis of variance (MANOVA), discriminant analysis and so forth—are founded on the eigenanalysis of covariance matrices.

[5] For real symmetric matrices the normalization is $E_{W,N}(H_{ij}^2) = \frac{1}{4}$, $1 \leq i < j \leq N$ and for complex hermitian matrices $\mathbb{E}_{W,N}(\mathrm{Re}(H_{ij})^2) = \mathbb{E}_{W,N}(\mathrm{Im}(H_{ij})^2) = \frac{1}{8}$.

Thus it is not surprising that the methods of random matrix theory have important applications to multivariate statistical analysis. We now survey some of these recent developments drawing heavily on Johnstone's 2006 ICM lecture [21]. We have also benefited from the unpublished survey by Péché [28].

3.1 Principal Component Analysis (PCA)

Recall that in PCA with p variables one distinguishes between the *population eigenvalues* ℓ_j, which are the eigenvalues of the underlying $p \times p$ covariance matrix

$$\Sigma = (\mathrm{Cov}(X_k, X_{k'}))_{1 \le k,k' \le p},$$

and the *sample eigenvalues* $\hat{\ell}_j$, which are the (random) eigenvalues of the sample covariance matrix

$$S = \frac{1}{n} X X^T.$$

Here X is the $p \times n$ data matrix and n is the number of observations of the p variables. (A column of X represents one observation of the p variables.) Since the parameters of the underlying probability model describing the random variables $X_1, \ldots, X_p$ are unknown, the problem is to deduce properties of Σ from the observed sample covariance matrix S.

The simplest model is to assume $\mathbb{X} = (X_1, \ldots, X_p)$ is a p-variate Gaussian distribution $N_p(\mu, \Sigma)$ and the data matrix X is formed by n independent draws $\mathbb{X}_1, \ldots, \mathbb{X}_n$. (For simplicity we consider $\mu = 0$.) The $p \times p$ matrix $A = XX^T$ is said to have p-variate *Wishart distribution* on n degrees of freedom, $W_p(n, \Sigma)$. We denote the eigenvalues of A by $l_1 \ge l_2 \ge \cdots l_p \ge 0$ (so $l_j = n\hat{\ell}_j$). The joint distribution of the eigenvalues l_j has been known for some time (e.g. Muirhead [24], Theorem 3.2.18) and is complicated by the fact it involves an integral over the orthogonal group $\mathbb{O}(p)$.

3.2 Testing the Null Hypothesis

The null hypothesis H_0 is the statement that there are no correlations amongst the p variables, i.e. $\Sigma = I$. Under H_0 all the population eigenvalues equal one, but as been known for some time[6] there is a "spread" in the sample eigenvalues $\hat{\ell}_j$. To assess whether "large" observed eigenvalues justify rejecting the null hypothesis, we need an approximation to the *null hypothesis distribution* of the largest sample eigenvalue,

[6] For $\Sigma = I$, the density of eigenvalues of S follows the Marchenko-Pastur distribution, a generalization of the Wigner semicircle distribution.

$$\mathbb{P}\left(\hat{\ell}_1 > t | H_0 = W_p(n, I)\right). \tag{7}$$

This approximation is provided by the following theorem of Johnstone [20].

Theorem 3.

$$\mathbb{P}\left(n\hat{\ell}_1 \leq \mu_{np} + \sigma_{np}x | H_0\right) \to F_1(x)$$

where the limit is $n \to \infty$, $p \to \infty$ such that $p/n \to \gamma \in (0, \infty)$, F_1 is the largest eigenvalue distribution (4)*, and the centering and norming constants are*

$$\mu_{np} = \left(\sqrt{n - \frac{1}{2}} + \sqrt{p - \frac{1}{2}}\right)^2, \tag{8}$$

$$\sigma_{np} = \left(\sqrt{n} + \sqrt{p}\right)\left(\frac{1}{\sqrt{n - \frac{1}{2}}} + \frac{1}{\sqrt{p - \frac{1}{2}}}\right)^{1/3}. \tag{9}$$

Several remarks are in order.

1. The appearance of the fractions $\frac{1}{2}$ in μ_{np} and σ_{np} appear to improve the rate of convergence to F_1 to "second-order accuracy" [21]. With this choice of constants, F_1 provides a good approximation for rather small values of p. (See Johnstone's comparisons with the tables of Chen [21].)
2. El Karoui [14] shows the theorem holds more generally as

$$p/n \to \gamma \in [0, \infty].$$

3. For complex data matrices with $\Sigma = I$, there are corresponding limit theorems where now convergence is to F_2 [18, 20].
4. Soshnikov [34] and Péché [27] have removed the assumption of Gaussian samples. They assume that the matrix elements X_{ij} of the data matrix X are independent random variables with a common symmetric distribution whose moments grow not faster than the Gaussian ones. We refer the reader to [27] for a description of the centering and norming constants. Limit theorems for complex data matrices are also proved.
5. To summarize, given the centering and norming constants (8) and (9) together with tables such as Table 2, one has a good approximation to the null distribution function (7).

3.3 Spiked Populations: BBP Phase Transition

As mentioned above, an essential difficulty in extending the above limit laws for $\hat{\ell}_1$ when the $A = XX^T \in W_p(n, \Sigma)$, $\Sigma \neq I$, is the presence of a certain integral over the orthogonal group $\mathbb{O}(p)$ in the joint distribution of eigenvalues of A. In the case of *complex* Wishart matrices, the corresponding integral in the joint distribution

Table 2 Values of x for given $\mathbb{P}(\chi_1 \geq x)$ where χ_1 has distribution F_1

x	$\mathbb{P}(\chi_1 \geq x)$
2.02345	0.01
1.59776	0.02
1.33321	0.03
1.13706	0.04
0.97931	0.05
0.84633	0.06
0.73069	0.07
0.62792	0.08
0.53508	0.09
0.45014	0.10

of eigenvalues is over the unitary group $\mathbb{U}(p)$ which, fortunately, can be explicitly evaluated by use of the Harish-Chandra-Itzykson-Zuber formula, see, e.g. [41].

We now describe the limit theorem of Baik, Ben Arous and Péché [3] where they consider the *complex* Wishart ensemble with the $p \times p$ covariance matrix

$$\Sigma = \operatorname{diag}(\ell_1, \ldots, \ell_r, 1, \ldots, 1)\,.$$

For ease of exposition of their results, we consider $r = 1$ with $\ell_1 > 1$. As before we consider the limit

$$p \to \infty, \qquad n \to \infty \quad \text{such that } \frac{p}{n} \to \gamma \geq 1. \tag{10}$$

Define

$$w_c = 1 + \sqrt{\gamma}.$$

Theorem 4. *With Σ as above ($r = 1$), let $\hat{\ell}_1$ denote the largest eigenvalue of the sample covariance matrix.*

- *If $1 \leq \ell_1 < w_c$, then in the limit (10)*

$$\mathbb{P}\left(\frac{n^{2/3}}{\sigma}\left(\hat{\ell}_1 - \mu\right) \leq x\right) \to F_2(x),$$

where F_2 is given by (2) and

$$\mu = (1 + \sqrt{\gamma})^2, \qquad \sigma = (1 + \sqrt{\gamma})\left(1 + \frac{1}{\sqrt{\gamma}}\right)^{1/3}.$$

- *If $\pi_1 > w_c$, then in the limit (10)*

$$\mathbb{P}\left(\frac{n^{1/2}}{\sigma_1}\left(\hat{\ell}_1 - \mu_1)\right) \leq x\right) \to \Phi(x),$$

where Φ is the standard normal distribution and

$$\mu_1 = \ell_1 \left(1 + \frac{\gamma}{\ell_1 - 1}\right), \qquad \sigma_1 = \ell_1^2 \left(1 - \frac{\gamma}{(\ell_1 - 1)^2}\right).$$

Remarks:

1. The BBP theorem "shows that a single eigenvalue of the true covariance Σ may drastically change the limiting behavior of the largest eigenvalue of sample covariance matrices. One should understand the above result as the statement that the eigenvalues exiting the support of the Marchenko-Pastur distribution form a small bulk of eigenvalues. This small bulk exhibits the same eigenvalue statistics as the eigenvalues of a non-normalized GUE (resp. GOE) matrix" [28].
2. If $\pi_1 = w_c$ the limiting distribution is a generalization of F_2 expressible in terms of the same Painlevé II function q [1].
3. For real Wishart matrices, Paul [26] shows that if $\pi_1 > w_c$ is simple, then $\hat{\ell}_1$ exhibits Gaussian fluctuations.
4. El Karoui [13] finds a large class of complex Wishart matrices $W_p(\Sigma, n)$ which have a F_2 limit law for $\hat{\ell}_1$.
5. Patterson, Price and Reich [25] have applied these results to problems of population structure arising from genetic data. See Harding [16] for an application in economics.

4 Conclusions

In this note we have surveyed some basic properties of the largest eigenvalue distributions F_β, their appearance as limit laws for large classes of random matrix models as well as their application to principal component analysis. We mention that these same distributions play an analogous role in canonical correlations [22] as they do in PCA.

We have not discussed the appearance of the F_β limit laws in *growth processes*. This line of research began with Baik, Deift & Johansson's work [2] on *Ulam's Problem* of the length of the longest increasing subsequence of a random permutation. (See also Johansson [18, 19] as well as [35] for a recent review.) Nor have we discussed the generalization of F_β to all real $\beta > 0$ by Ramírez, Rider and Virág [32].

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Hybrid Formalism and Topological Amplitudes

Jürg Käppeli, Stefan Theisen, and Pierre Vanhove

Abstract We study four-dimensional compactifications of type II superstrings on Calabi-Yau spaces in the hybrid formalism. Chiral and twisted-chiral interactions are rederived, which involve the coupling of the compactification moduli to two powers of the Weyl-tensor and of the derivative of the universal tensor field-strength. We review the formalism and provide details of some of its technicalities.

1 Introduction

Type II string compactified on a Calabi–Yau 3-fold gives rise to $\mathcal{N} = 2$ supergravity in four dimension. Most calculations of string scattering amplitudes, and therefore of the construction of the low-energy-effective action, are based on the Ramond-Neveu-Schwarz (RNS) formulation of the superstring. A drawback of this formulation is that spacetime supersymmetry is not manifest and is achieved only after GSO projection.

An alternative formulation without these complications is the hybrid formulation. Hybrid string theory can be obtained by a field redefinition from the gauge-fixed RNS string or by covariantizing the Green-Schwarz (GS) string in light-cone gauge. In this sense, worldsheet reparametrizations are gauge-fixed in the hybrid formulation. Nevertheless, there is no need for ghost-like fields in the formalism since the theory can be formulated as a $\mathcal{N} = 4$ topological theory and amplitudes

Jürg Käppeli
Institut für Physik, Humboldt Universität, Berlin, Germany, e-mail: kaeppeli@aei.mpg.de

Stefan Theisen
Max-Planck-Institut für Gravitationsphysik, Albert-Einstein-Institut, Golm, Germany, e-mail: theisen@aei.mpg.de

Pierre Vanhove
CEA/DSM/SPhT, URA au CNRS, CEA/Saclay, 91191 Gif-sur-Yvette, France, e-mail: pierre.vanhove@cea.fr

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can be computed directly by the methods of topological string theory [12]. The theory consists of two completely decoupled twisted worldsheet SCFT, one describing the spacetime part, one the internal part. Despite being twisted, hybrid string theory describes the full theory, i.e., it computes also non-topological amplitudes. Hybrid type IIA and IIB string theories are distinguished by the relative twisting of the left- and right-moving sector of the internal SCFT. When working with either type one is therefore committed to a given fixed twisting.

The hybrid formulation was developed in a series of papers by N. Berkovits and various collaborators [12, 7, 10]. It was reviewed in [9]. One purpose of this note is our attempt to fill in details of some of the more technical aspects. This is done in Sect. 2 and the Appendices B and C, the content of which is well known to the few experts in the field, but often not readily accessible.

The main application of hybrid strings in this note are presented in Sects. 3 and 4. We extend the analysis of higher order derivative interactions to the twisted-chiral sector. The procedure is analogous to the computation in the chiral sector given [12]. Even though one is working with a fixed relative twisting, giving rise to either type IIA or type IIB, it is shown that the chiral and twisted-chiral couplings of each type II theory depend on both the A-model and B-model topological partition functions. In the effective action these amplitudes give rise to couplings of compactification moduli to two powers of the Weyl tensor or of the derivative of the universal tensor field-strength. In the RNS formulation these couplings were discussed in [4].

Another possible application is flux compactifications of the type II string with $\mathcal{N} = 1$ spacetime supersymmetry. The breaking $\mathcal{N} = 2 \to \mathcal{N} = 1$ results from auxiliary fields acquiring vacuum expectation values [30]. Due to its manifest spacetime supersymmetry, the hybrid formulation might be the most suitable. First steps in this direction were already taken in [24, 26].

2 Compactified String Theory in RNS and Hybrid Variables

In this section we present a detailed account of the field mapping between the variables of the Ramond-Neveu-Schwarz (RNS) formulation of those of the hybrid formulation of the superstring. We consider here only Calabi-Yau compactifications to four spacetime dimensions and split all variables into a spacetime and an internal part. The internal part is practically the same for the RNS and the hybrid formulation, while the two descriptions of the spacetime are different.

2.1 Hybrid Variables

Type II and heterotic string theory compactified on a Calabi-Yau three-fold can be formulated within a covariant version of the Green-Schwarz (GS) formulation [7, 10]. The spacetime part consists of four bosons x^m, two pairs of left-moving canon-

ically conjugate Weyl fermions (p_α, θ^β) and $(\bar{p}^{\dot\alpha}, \bar\theta_{\dot\beta})$, both of conformal weight $(1, 0)$ and a chiral boson ρ with action

$$S = \frac{1}{\pi}\int d^2z \left\{\frac{1}{2}\bar\partial x^m \partial x_m + p^\alpha \bar\partial\theta_\alpha + \bar p_{\dot\alpha}\bar\partial\bar\theta^{\dot\alpha} + \tilde p^\alpha \partial\tilde\theta_\alpha + \tilde{\bar p}_{\dot\alpha}\partial\tilde{\bar\theta}^{\dot\alpha} + \frac{1}{2}\bar\partial\rho\partial\rho\right\}. \tag{1}$$

The chiral boson is periodic with period $\rho \sim \rho + 2\pi i$ and

$$\rho(z)\rho(w) = -\ln(z-w). \tag{2}$$

From these fields one constructs the generators

$$\begin{aligned} T &= -\frac{1}{2}\partial x^m\partial x_m - p^\alpha\partial\theta_\alpha - \bar p_{\dot\alpha}\partial\bar\theta^{\dot\alpha} - \frac{1}{2}\partial\rho\partial\rho - \frac{1}{2}Q_\rho\partial^2\rho,\\ G^- &= \frac{1}{\sqrt{32}}e^\rho\, d^2, \qquad G^+ = -\frac{1}{\sqrt{32}}e^{-\rho}\,\bar d^2,\\ J &= \partial\rho. \end{aligned} \tag{3}$$

We have defined the fermionic currents (cf. Appendix A)

$$\begin{aligned} d_\alpha &= p_\alpha + i\bar\theta^{\dot\alpha}\partial x_{\alpha\dot\alpha} - \bar\theta^2\partial\theta_\alpha + \frac{1}{2}\theta_\alpha\partial\bar\theta^2,\\ \bar d^{\dot\alpha} &= \bar p^{\dot\alpha} + i\theta_\alpha\partial x^{\alpha\dot\alpha} - \theta^2\partial\bar\theta^{\dot\alpha} + \frac{1}{2}\bar\theta^{\dot\alpha}\partial\theta^2. \end{aligned} \tag{4}$$

In the definition of the energy-momentum tensor a background charge Q_ρ for the chiral boson ρ is included. It is obtained from the coupling of the field ρ to the world-sheet curvature. This coupling is not visible in conformal gauge. The background charge implies the conformal weights $\mathrm{wt}(\exp(q\rho)) = -\frac{1}{2}q(q+Q_\rho)$, and therefore $\mathrm{wt}(\exp(\pm\rho)) = -\frac{1}{2}(1\pm Q_\rho)$ and $\mathrm{wt}(G^\pm) = \frac{1}{2}(3\pm Q_\rho)$. Also the central charge of the Virasoro algebra depends on the value of Q_ρ. It is $c_x + c_{p,\theta} + c_{\bar p,\bar\theta} + c_\rho = 4-4-4+(1+3Q_\rho^2) = 3(Q_\rho^2-1)$. For $Q_\rho = 0$, (T, G^+, G^-, J) generate an untwisted $c=-3$, $\mathscr{N}=2$ superconformal algebra while for non-vanishing Q_ρ the algebra is twisted. It is topological for $Q_\rho = \pm 1$. When checking the algebra for this case, in particular, the correct overall sign on the right-hand side of

$$G^+(z)G^-(w) \sim \frac{\frac{c}{3}}{(z-w)^3} + \frac{J(w)}{(z-w)^2} + \frac{T(w)}{z-w}, \tag{5}$$

for $c=-3$, the relative minus sign in the definitions of $G^\pm$ is crucial. It is also consistent with the requirement $(G^+)^\dagger = G^-$ if we define $(e^\rho)^\dagger = -e^{-\rho}$. The hermiticity properties of the hybrid variables are further discussed in Appendices A and B. As explained in Sect. 2.3, the field mapping from the RNS variables determines the background charge as $Q_\rho = -1$. The four-dimensional part is therefore a twisted $c=-3$, $\mathscr{N}=2$ superconformal algebra.

The Calabi-Yau compactification is described by an internal $\mathcal{N}=2$ SCFT. The generators (T_C, G_C^+, G_C^-, J_C) form an untwisted $c=9$, $\mathcal{N}=2$ superconformal algebra and commute with (3). The generators $(\mathscr{T}, \mathscr{G}^\pm, \mathscr{J})$ of the combined system are obtained by adding[1] the twisted generators $(T_C + \frac{1}{2}\partial J_C, G_C^+, G_C^-, J_C)$ to those of (3),

$$\mathscr{T} = T + T_C + \frac{1}{2}\partial J_C, \quad \mathscr{G}^\pm = G^\pm + G_C^\pm, \quad \mathscr{J} = J + J_C. \tag{6}$$

They form a twisted $c=6$, $\mathcal{N}=2$ superconformal algebra. The current J_C can be represented in terms of a free boson H as $J_C = i\sqrt{3}H$. The generators $G_C^\pm$ can then be written in the form $G_C^+ = e^{+\frac{i}{\sqrt{3}}H} G'$ and $G_C^- = e^{-\frac{i}{\sqrt{3}}H} \bar{G}'$ where G' and $\bar{G}'$ are uncharged under J_C. The conformal weight of $e^{\frac{iq}{\sqrt{3}}H}$ is $\frac{q}{6}(q-3)$.

For a twisted algebra, the conformal anomaly vanishes (though the other currents are anomalous). There are, therefore, two options: either, one untwists the resulting algebra, couples the system to a set of $c=-6$, $\mathcal{N}=2$ superconformal ghosts (thereby canceling the central charge) and calculates scattering amplitudes utilizing the $\mathcal{N}=2$ prescription [6]. Alternatively, one embeds the twisted $c=6$, $\mathcal{N}=2$ SCFT into a (small version of the) twisted $\mathcal{N}=4$ algebra and uses the topological prescription [12, 14] to compute the spectrum and correlation functions. This is the method we follow.

The embedding into a twisted small $\mathcal{N}=4$ superconformal algebra[2] proceeds as follows: The U(1)-current $\mathscr{J} = J + J_C$ is augmented to a triplet of currents $(\mathscr{J}^{++}, \mathscr{J}, \mathscr{J}^{--})$. The $\mathscr{J}$-charge of $\mathscr{J}^{\pm\pm}$ is ± 2 and the conformal weights are $\mathrm{wt}(\mathscr{J}^{++}) = 0$ and $\mathrm{wt}(\mathscr{J}^{--}) = 2$. They satisfy the SU(2) relation

$$\mathscr{J}^{++}(z)\,\mathscr{J}^{--}(w) \sim \frac{1}{(z-w)^2} + \frac{\mathscr{J}(w)}{(z-w)}. \tag{7}$$

There are two SU(2) doublets of fermionic generators: $(\mathscr{G}^+, \widetilde{\mathscr{G}}^-)$ and $(\mathscr{G}^-, \widetilde{\mathscr{G}}^+)$ that transform in the **2** and $\mathbf{2}^*$ of SU(2), respectively. The $\widetilde{\mathscr{G}}^\pm$ are defined via the operator products

$$\mathscr{J}^{\pm\pm}(z)\mathscr{G}^\mp(w) \sim \mp\frac{\widetilde{\mathscr{G}}^\pm(w)}{z-w}, \quad \mathscr{J}^{\pm\pm}(z)\widetilde{\mathscr{G}}^\mp(w) \sim \pm\frac{\mathscr{G}^\pm(w)}{z-w} \tag{8}$$

and have $\mathrm{wt}(\tilde{\mathscr{G}}^+) = 1$ and $\mathrm{wt}(\tilde{\mathscr{G}}^-) = 2$. The other OPEs of $\mathscr{J}^{\pm\pm}$ with the fermionic generators are finite. The notation $\widetilde{\mathscr{O}}$ refers to a more general operator conjugation $\mathscr{O} \to \widetilde{\mathscr{O}}$, for which (8) is a special case. It is explained in Appendix B.

The nontrivial OPEs of the supercurrents are

[1] When working with the explicit realizations (3) of $G^\pm$ cocycle factors must be included in order for the space-time and the internal part of $\mathscr{G}^\pm$ to anticommute. The explicit expressions are given in (12).

[2] Small $\mathcal{N}=4$ superconformal algebras were constructed in [2, 3]. Our conventions are based on the algebra presented in [35].

$$\begin{aligned}\mathscr{G}^+(z)\widetilde{\mathscr{G}}^+(w) &\sim \frac{2\mathscr{J}^{++}(w)}{(z-w)^2}+\frac{\partial\mathscr{J}^{++}(w)}{z-w},\\ \widetilde{\mathscr{G}}^-(z)\mathscr{G}^-(w) &\sim \frac{2\mathscr{J}^{--}(w)}{(z-w)^2}+\frac{\partial\mathscr{J}^{--}(w)}{z-w}\end{aligned} \tag{9}$$

and

$$\mathscr{G}^+(z)\mathscr{G}^-(w) \sim \frac{2}{(z-w)^3}+\frac{\mathscr{J}(w)}{(z-w)^2}+\frac{\mathscr{T}(w)}{z-w}, \tag{10}$$

and the very same OPE for $\widetilde{\mathscr{G}}^+(z)$ and $\widetilde{\mathscr{G}}^-(w)$. The explicit form of the currents and super-currents is

$$\mathscr{J}^{\pm\pm}(z) = c_\pm e^{\pm\int^z\mathscr{J}} = c_\pm e^{\pm(\rho+i\sqrt{3}H)}, \tag{11}$$

and

$$\begin{aligned}\mathscr{G}^+ &= -\left(\frac{1}{\sqrt{32}}e^{-\rho}\bar{d}^2+c_+G_C^+\right)\\ \mathscr{G}^- &= \frac{1}{\sqrt{32}}e^{\rho}d^2+c_-G_C^-\\ \tilde{\mathscr{G}}^+ &= -\left(\frac{1}{\sqrt{32}}c_+e^{2\rho+i\sqrt{3}H}d^2+e^{\rho}G_C^{++}\right)\\ \tilde{\mathscr{G}}^- &= -\left(\frac{1}{\sqrt{32}}c_-e^{-2\rho-i\sqrt{3}H}\bar{d}^2+e^{-\rho}G_C^{--}\right)\end{aligned} \tag{12}$$

Here $G_C^{\pm\pm}$ are defined[3] as $G_C^{\pm\pm} = e^{\pm i\sqrt{3}H}(G_C^{\mp})$ and $c_\pm = e^{\pm i\pi\oint\mathscr{J}} = e^{\pm i\pi(p_\rho+\sqrt{3}p_H)}$.[4] The various signs and cocycle factors $c_\pm$ are necessary in order to guarantee the hermiticity relations $(\mathscr{J}^{++})^\dagger = \mathscr{J}^{--}$, $(\mathscr{G}^+)^\dagger = \mathscr{G}^-$ and $(\tilde{\mathscr{G}}^+)^\dagger = \tilde{\mathscr{G}}^-$, the appropriate Grassmann parity of the generators, and for correctly reproducing the algebra.

In type II theories the spacetime fields are supplemented by two pairs of right-moving canonically conjugate Weyl fermions and a periodic right-moving chiral boson. We will use the subscripts "L" and "R" in order to distinguish left-moving from right-moving fields and adopt the notation $|A|^2 = A_LA_R$. For notational simplicity we discuss mostly type IIB string theory, for which the left- and right-movers are twisted in the same way. For type IIA theories the right-moving part of the algebra is obtained by the opposite twisting as compared to IIB. Operationally, the expressions for IIA can be obtained from those of IIB by replacing $(J_C)_R \to -(J_C)_R$ (thereby reversing the background charge) in above definitions of the currents and by reversing, e.g., $(G_C^\pm)_R \to (G_C^\mp)_R$. The spacetime part remains unaffected.

[3] The expression $A(B(w))$ denotes the residue in the OPE of $A(z)$ with $B(w)$ and equals the (anti)commutator $[\oint A, B(w)\}$. The notation is $\oint A \equiv \frac{1}{2\pi i}\oint dzA(z)$.

[4] The momentum modes $p_\rho = \oint\partial\rho$ and $p_H = i\oint\partial H$ satisfy the commutation relations $[p_\rho,\rho] = -1$ and $[p_H, H] = -i$. Their hermiticity properties are discussed in Appendix B and imply $(c_+)^\dagger = c_-$.

2.2 RNS Variables

In the RNS representation the spacetime fields are (x^m, ψ^m) with $m = 1, \ldots, 4$. They contribute with $c^{x,\psi} = 6$ to the central charge of the Virasoro algebra. We will concentrate on the left-moving sector in what follows.

It is convenient to bosonize the (Euclideanized) worldsheet fermions,

$$\psi^1 \pm i\psi^2 = e^{\pm i\varphi^1}, \qquad \psi^3 \pm i\psi^4 = e^{\pm i\varphi^2}. \tag{13}$$

As usual we suppress cocycle factors. The bosonized expression for the SO(4)-spin fields of positive and negative chirality are

$$S^\alpha = e^{\pm\frac{i}{2}(\varphi^1+\varphi^2)}, \qquad \bar{S}^{\dot\alpha} = e^{\pm\frac{i}{2}(\varphi^1-\varphi^2)}. \tag{14}$$

The internal sector (the Calabi-Yau threefold) is accounted for by a $c = 9$ CFT with $\mathcal{N} = 2$ worldsheet superconformal symmetry generated by $\breve{T}_C$, $\breve{G}_C{}^\pm$, and $\breve{J}_C$. Their relation to the generators introduced in the previous section is explained in Sect. 2.3. The U(1) R-current $\breve{J}_C$ can be expressed in terms of a free chiral boson $\breve{H}$ as

$$\breve{J}_C = i\sqrt{3}\partial\breve{H}, \quad \breve{H}(z)\breve{H}(w) = -\ln(z-w). \tag{15}$$

Any field $\mathcal{O}^{(q)}$ with R-charge q can be decomposed as $\mathcal{O}^{(q)} = \exp(\frac{iq}{\sqrt{3}}\breve{H})\mathcal{O}'$ where $\mathcal{O}'$ is uncharged with respect to $\breve{J}_C$. For the generators $\breve{G}_C^\pm$ this part is independent of $\breve{H}$.

Covariant quantization requires fixing the local reparametrization invariance of $\mathcal{N} = 1$ worldsheet supergravity. This introduces the (b, c) and (β, γ) ghost systems. With $c^{\rm gh} = -15$ the total central charge vanishes. Following [23], we 'bosonize' the ghosts

$$\begin{aligned} b &= e^{-\sigma}, & c &= e^{\sigma}, \\ \beta &= e^{-\varphi}\partial\xi = e^{-\varphi+\chi}\partial\chi, & \gamma &= e^{\varphi}\eta e^{\varphi-\chi}, \\ \xi &= e^{\chi}, & \eta &= e^{-\chi}. \end{aligned} \tag{16}$$

The total energy-momentum tensor is

$$\begin{aligned} T_{\rm RNS} = &-\frac{1}{2}\partial x^m \partial x_m - \frac{1}{2}\psi^m\partial\psi_m + \breve{T}_C \\ &+ \frac{1}{2}\Big[(\partial\sigma)^2 + (\partial\chi)^2 - (\partial\varphi)^2\Big] - \frac{1}{2}\partial^2(2\varphi - 3\sigma - \chi). \end{aligned} \tag{17}$$

The generators $(T_{\rm RNS}, b, j_{\rm BRST}, J^{\rm gh})$ form a twisted $\mathcal{N} = 2$ algebra. The U(1)-current is $J^{\rm gh} = -(bc + \xi\eta)$. The BRST-current $j_{\rm BRST}$ is given in Appendix B.

2.3 Field Redefinition from RNS to Hybrid Variables

The RNS variables are mapped to the hybrid variables in a two-step procedure. From the RNS variables one first forms a set of variables, called the "chiral GS-variables" in [7, 12]. In this section, we refer to these variables. The hybrid variables of the previous section are obtained in a second step by performing a field redefinition on the chiral GS-variables. We will suppress this field redefinition in the following and refer to Appendix B for a detailed account.

Following [7, 12] we define the following superspace variables:[5]

$$\begin{aligned} \theta^\alpha &= c\xi e^{-\frac{3}{2}\varphi}\bar{\Sigma}S^\alpha, \qquad & \bar{\theta}^{\dot\alpha} &= e^{\frac{\varphi}{2}}\Sigma\bar{S}^{\dot\alpha}, \\ p_\alpha &= b\eta e^{\frac{3}{2}\varphi}\Sigma S_\alpha, & \bar{p}_{\dot\alpha} &= e^{-\frac{\varphi}{2}}\bar{\Sigma}\bar{S}_{\dot\alpha}, \end{aligned} \tag{18}$$

where

$$\Sigma = e^{\frac{i}{2}\sqrt{3}\check{H}}, \quad \bar{\Sigma} = e^{-\frac{i}{2}\sqrt{3}\check{H}}. \tag{19}$$

In this definition, θ^α (p_α) carries charge $q_C = -\frac{3}{2}$ ($+\frac{3}{2}$). Here and in the following, q_C denotes the charge under $\oint \check{J}_C$, the U(1) R-symmetry of the internal $c = 9$ SCFT.

In order to implement a complete split between the spacetime and the internal part one must require that the hybrid variables (18) do not transform under the $c = 9$ SCFT generators. For instance, the variables (18) should not carry a charge with respect to the U(1) R-symmetry. This can be realized by shifting the U(1) charge by the picture-counting operator,

$$\mathscr{P} = -\beta\gamma + \xi\eta = -\partial\varphi + \partial\chi. \tag{20}$$

The variable θ^α, for instance, has picture $-\frac{1}{2}$. This motivates the following definition of the shifted U(1) current

$$J_C = \check{J}_C - 3\mathscr{P} = \check{J}_C + 3\partial(\varphi - \chi). \tag{21}$$

More generally, the fields of the internal part are transformed by the field transformation [7, 12]

$$F_C = e^{\mathscr{W}}\check{F}_C e^{-\mathscr{W}}, \quad \mathscr{W} = \oint (\varphi - \chi)\check{J}_C. \tag{22}$$

For the other generators of the internal $\mathscr{N} = 2$ algebra this implies

$$\begin{aligned} G_C^+ &= e^{(\varphi-\chi)}\check{G}_C^+, \\ G_C^- &= e^{-(\varphi-\chi)}\check{G}_C^-, \\ T_C &= \check{T}_C + \partial(\varphi - \chi)\check{J}_C + \frac{3}{2}(\partial\varphi - \partial\chi)^2. \end{aligned} \tag{23}$$

[5] The RNS variables are actually subject to the rescaling given in Appendix B.1. We neglect this issue here.

These are the generators that couple to the chiral GS-variables defined in (18). The generators coupling to the hybrid variables are related to these by the field redefinition discussed in Appendix B, which does not affect the algebraic structure discussed in the following. The currents (T_C, G_C^+, G_C^-, J_C) generate an untwisted $\mathcal{N} = 2$ superconformal algebra. The shift by the picture changing current in the relation (21) amounts to a background charge $Q_{J_C} = -3$ for the current J_C. The RNS ghost-current

$$J^{\text{gh}} = -(bc + \xi\eta) = \partial\sigma - \partial\chi, \tag{24}$$

which is obtained from the ghost current of the "small Hilbert space" $-(bc+\beta\gamma) = \partial\sigma - \partial\varphi$ by adding the picture-counting operator (20), is mapped to a combination of the current $J = \partial\rho$ and the shifted internal U(1) R-current [7, 12],

$$J = \partial\rho = J^{\text{gh}} - J_C = \partial\sigma + 2\partial\chi - 3\partial\varphi - \check{J}_C. \tag{25}$$

This equation defines the chiral boson ρ in terms of the RNS variables. The mapping is such that the ρ-system[6] acquires a background charge $Q_\rho = -1$ and that it has regular OPEs with the internal generators (T_C, G_C^+, G_C^-, J_C). The superspace variables θ, $\bar{\theta}$, p and $\bar{p}$, and the redefined internal operators (22) all have zero ρ-charge. This, in particular, means that (22) leads to a complete decoupling of the internal sector from the chiral GS-variables.

The field redefinitions (18) are such that the RNS generators $(T_{\text{RNS}}, b, j_{\text{BRST}}, J^{\text{gh}})$ map to the hybrid generators of the $\mathcal{N} = 2$ algebra

$$T_{\text{RNS}} = \mathscr{T}, \quad b = \mathscr{G}^-, \quad j_{\text{BRST}} = \mathscr{G}^+, \quad J^{\text{gh}} = \mathscr{J}. \tag{26}$$

We hasten to add that in order to arrive at this correspondence one must correctly take into account the field mapping from the chiral GS-variables to the hybrid variables (cf. Appendix B).

It is straightforward to express the raising and lowering operators (11) of the $\mathcal{N} = 4$ algebra in terms of RNS variables, since one can verify that these are not affected by the additional field redefinition, mapping hybrid to chiral GS-variables as discussed in Appendix B. From (18) one therefore concludes

$$\mathscr{J}^{++} = c\eta, \qquad \mathscr{J}^{--} = b\xi. \tag{27}$$

Using this it is easy to verify that the generators $\widetilde{\mathscr{G}}^{\pm}$, defined through (8), are expressed in RNS variables by

$$\widetilde{\mathscr{G}}^- = [Q_{\text{BRST}}, b\xi] = Z + \xi T_{\text{RNS}}, \quad \widetilde{\mathscr{G}}^+ = \eta, \tag{28}$$

where Z is the picture changing operator of the RNS formalism, given in (B.20). We summarize the dictionary between the RNS and the hybrid currents in the following table:

[6] The current which satisfies $T(z)j(w) \sim \frac{Q_\rho}{(z-w)^3} + \cdots$ and leads to $\bar{\partial} j = \frac{1}{8} Q_\rho \sqrt{g} R$ is $j = -\partial\rho = -J$.

$$\begin{aligned} \mathscr{T} &= T_{\mathrm{RNS}}, \\ \mathscr{J}^{++} &= c\eta, \quad \mathscr{J}^{--} = b\xi, \quad \mathscr{J} = J^{\mathrm{gh}} = -(bc + \xi\eta), \\ \mathscr{G}^{+} &= j_{\mathrm{BRST}}, \quad \widetilde{\mathscr{G}}^{+} = \eta, \quad \mathscr{G}^{-} = b, \quad \widetilde{\mathscr{G}}^{-} = bZ + \xi T_{\mathrm{RNS}}. \end{aligned} \tag{29}$$

So far we have concentrated on the left-moving (holomorphic) sector of the theory. For the heterotic string the right-moving sector is treated in the same way as in the RNS formulation: it is simply the bosonic string. For the type II string, however, the distinction between type IIA and IIB needs to be discussed. Since the construction presented above involves twisting the internal $c = 9$ SCFT, the distinction between IIA and IIB is analogous to the one in topological string theory where one deals with the so-called A and B twists (which are related by mirror symmetry). In type IIB, the left- and right-moving sectors are treated identically and the distinction is merely in the notation, i.e., to replace all fields $\varphi_L(z)$ by $\varphi_R(\bar{z})$. In type IIA, however, the twists in the two sectors are opposite. The two possible twists differ in the shift of the conformal weight, which is either $h \to h - \frac{1}{2}q$ or $h \to h + \frac{1}{2}q$. Above we have discussed the first possibility. The second twist is implemented by the replacement $\breve{T}_C \to \breve{T}_C - \frac{1}{2}\partial\breve{J}_C$ and follows from the first by the substitution $\breve{J}_C \to -\breve{J}_C$. This also implies that the transformation (22) is now defined with $\mathscr{W} = -\oint(\varphi - \chi)\breve{J}_C$ which leads to

$$\begin{aligned} T_C &= \breve{T}_C - \partial(\varphi - \chi)\breve{J}_C + \frac{3}{2}(\partial\varphi - \partial\chi)^2, \\ J_C &= \breve{J}_C + 3\mathscr{P}, \end{aligned} \tag{30}$$

and

$$J = \partial\rho = J^{\mathrm{gh}} + J_C = \partial\sigma + 2\partial\chi - 3\partial\varphi + \breve{J}_C. \tag{31}$$

With this definition, ρ still has background charge $Q_\rho = -1$. The twisted $c = 9$ SCFT is generated by $(T_C - \frac{1}{2}\partial J_C, G_C^+, G_C^-, J_C)$, where now the conformal weights of G_C^+ and G_C^- are two and one, respectively. The full right-moving supersymmetry generators for the type IIA theory are (suppressing signs and cocycle factors)

$$\mathscr{G}_R^{\pm} = G_R^{\pm} + G_{CR}^{\mp}. \tag{32}$$

The map between RNS and hybrid variables must also be modified for the latter to be neutral under J_C:

$$\begin{aligned} \theta^\alpha &= c\xi e^{-\frac{3}{2}\varphi}\Sigma S^\alpha, \qquad \bar{\theta}^{\dot{\alpha}} = e^{\frac{\varphi}{2}}\bar{\Sigma}\bar{S}^{\dot{\alpha}}, \\ p_\alpha &= b\eta e^{\frac{3}{2}\varphi}\bar{\Sigma}S_\alpha, \qquad \bar{p}_{\dot{\alpha}} = e^{-\frac{\varphi}{2}}\Sigma\bar{S}_{\dot{\alpha}}. \end{aligned} \tag{33}$$

In the type IIA theory this applies for the right-movers, given (18) for the left movers. Summarizing, the difference between type IIA and type IIB is seen in the different right-moving U(1) charge assignment to ρ_R.

2.4 Physical State Conditions and $\mathcal{N} = 4$-embeddings

Having the dictionary (29) at hand it is simple to rephrase the standard physical state conditions of the RNS formalism in terms of hybrid variables. We refer to [9, 14] for details. Physical RNS vertex operators are in the cohomology of $Q_{\text{BRST}} = \oint j_{\text{BRST}}$ and $\oint \eta$:

$$j_{\text{BRST}}(V^+) = 0, \quad \eta(V^+) = 0, \quad \delta V^+ = j_{\text{BRST}}(\eta(\Lambda^-)). \tag{34}$$

The condition imposed by $\oint \eta$ implies that V^+ is in the small RNS Hilbert space, i.e., it does not depend on the ξ zero-mode. Furthermore, V^+ has ghost number 1 with respect to (24) as indicated with the superscript. The charge with respect to $-(bc + \beta\gamma)$ is $1 + \mathscr{P}$, where $\mathscr{P}$ is the picture (20). Using (29), the conditions (34) are expressed in hybrid variables as

$$\mathscr{G}^+(V^+) = 0, \quad \widetilde{\mathscr{G}}^+(V^+) = 0, \quad \delta V^+ = \mathscr{G}^+(\widetilde{\mathscr{G}}^+(\Lambda^-)). \tag{35}$$

In addition, V^+ has $\mathscr{J}$-charge 1 as indicated. Note that $\mathscr{G}^+$ and $\widetilde{\mathscr{G}}^+$ have trivial cohomologies, since

$$\mathscr{G}^+\left(\sqrt{2}e^{\rho}\bar{\theta}^2\right) = 1, \quad \widetilde{\mathscr{G}}^+\left(\widetilde{\sqrt{2}(e^{\rho}\bar{\theta}^2)}\right) = 1. \tag{36}$$

Therefore, one can solve, e.g., the $\widetilde{\mathscr{G}}^+$-constraint by introducing the U(1)-neutral field $\mathscr{V}$ satisfying

$$V^+ = \widetilde{\mathscr{G}}^+(\mathscr{V}). \tag{37}$$

Up to the gauge transformations $\delta\mathscr{V} = \widetilde{\mathscr{G}}^+(\widetilde{\Lambda}^-)$, $\mathscr{V}$ is determined in terms of V^+ by $\mathscr{V} = \widetilde{\sqrt{2}(e^{\rho}\theta^2)}V^+$, where we used (36). It follows that (35) can be rephrased in terms of $\mathscr{V}$ as

$$\mathscr{G}^+(\widetilde{\mathscr{G}}^+(\mathscr{V})) = 0, \quad \delta\mathscr{V} = \mathscr{G}^+(\Lambda^-) + \widetilde{\mathscr{G}}^+(\widetilde{\Lambda}^-). \tag{38}$$

Using RNS variables these manipulations become much more transparent. Notice that $\widetilde{\sqrt{2}(e^{\rho}\bar{\theta}^2)} = e^{-2\rho - i\sqrt{3}H}\theta^2 = \xi$. The first equality follows from the definition (B.23), the second from (18) (the additional conjugation in Appendix B.2 does not affect this result). Therefore, $\mathscr{V}$ lives in the large RNS Hilbert space. Using the RNS variables it is straightforward to show that $\mathscr{G}^+(\mathscr{V}) = ZV^+ = Z\widetilde{\mathscr{G}}^+(\mathscr{V})$, hence $\mathscr{G}^+(\mathscr{V})$ and $\widetilde{\mathscr{G}}^+(\mathscr{V})$ are related by picture changing. This will play a role momentarily when we discuss integrated vertex operators. From now on we will often drop the bracket on expressions like $\mathscr{G}^{\pm}(\mathscr{V})$ when the generators $\mathscr{G}^{\pm}$ and alike are involved, i.e., $\mathscr{G}^{\pm}\mathscr{V} \equiv \mathscr{G}^{\pm}(\mathscr{V})$.

Following [14] we fix the gauge symmetry (38) by choosing a gauge condition which resembles Siegel gauge: we require the vanishing of the second-order poles in the OPE's of $\mathscr{G}^-$ and $\widetilde{\mathscr{G}}^-$ with $\mathscr{V}$. Vertex operators $\mathscr{V}$ in this gauge have conformal weight 0. For SU(2) singlets these gauge fixing conditions are equivalent to the

vanishing of the second-order poles of $\mathscr{G}^-$ and $\mathscr{G}^+$ with $\mathscr{V}$. For massless fields $\mathscr{V}(x,\theta,\bar{\theta})$ that depend only on x, θ^α, and $\bar{\theta}^{\dot{\alpha}}$ but not their derivatives, there are no poles of order 3 or higher in the OPE of $\mathscr{V}(x,\theta,\bar{\theta})$ with $\mathscr{G}^\pm$. Hence for these operators the gauge fixing constraints are equivalent to the primarity constraints of the $\mathscr{N}=2$ subalgebra, which here means the vanishing of all poles of order 2 and higher in the OPE of $\mathscr{V}$ with $\mathscr{G}^\pm$. This has also been explained in [9, 12, 10] and we will use these gauge-fixing constraints in the next sections also for massless fields that depend non-trivially on the compactification. So far we have discussed the unintegrated vertex operators V^+ and $\mathscr{V}$ residing in the small and large Hilbert spaces, respectively. To construct integrated vertex operators one proceeds like in the RNS formulation: $\int b(V^+) = \int \mathscr{G}^- V^+$. Note that for this choice the integrated and the unintegrated vertex operators are in the same picture $\mathscr{P}$. To obtain different pictures one considers $\int \widetilde{\mathscr{G}}^- V^+$. As is shown in [14], this provides the integrated vertex operator in a different ghost picture, $\int \widetilde{\mathscr{G}}^- V^+ = \int \mathscr{G}^-(Z_0 V^+)$. Expressing the operators V^+ in terms of $\mathscr{V}$ opens new though related possibilities: using the previous result that relates $\widetilde{\mathscr{G}}^+\mathscr{V}$ and $\mathscr{G}^+\mathscr{V}$, one concludes that the four possible integrated vertex operators, $\int \mathscr{G}^-\widetilde{\mathscr{G}}^+\mathscr{V}$, $\int \mathscr{G}^-\mathscr{G}^+\mathscr{V}$, $\int \widetilde{\mathscr{G}}^-\widetilde{\mathscr{G}}^+\mathscr{V}$, and $\int \widetilde{\mathscr{G}}^-\mathscr{G}^+\mathscr{V}$ are all related by picture changing.

In the next sections we will use the following canonical ghost pictures: we take the unintegrated NS- and R-vertex operators in the -1 and $-\frac{1}{2}$ picture, respectively, the integrated ones in the 0 and $+\frac{1}{2}$ picture. Therefore, the relevant prescription is

$$\int b(ZV^+) = \int \mathscr{G}^-\mathscr{G}^+\mathscr{V} = \int \widetilde{\mathscr{G}}^-\widetilde{\mathscr{G}}^+\mathscr{V} \tag{39}$$

Adding the right-moving sector, the relevant expression for the integrated vertex operators can be written as

$$\int d^2z \mathscr{W}(z,\bar{z}) = \int d^2z \left|\mathscr{G}^-\mathscr{G}^+\right|^2 \mathscr{V}(z,\bar{z}). \tag{40}$$

For better readability we drop the parenthesis here and in the following when the first-order poles in OPE with the generators $\mathscr{G}^\pm$ and alike are meant.

It is convenient to label the fermionic generators by indices $i, j 1, 2$ according to

$$\mathscr{G}_i^+ = (\mathscr{G}^+, \widetilde{\mathscr{G}}^+), \qquad \mathscr{G}_i^- = (\mathscr{G}^-, \widetilde{\mathscr{G}}^-). \tag{41}$$

They satisfy the hermiticity property $(\mathscr{G}_i^+)^\dagger \mathscr{G}_i^-$. Consider general linear combinations

$$\widehat{\mathscr{G}}_i^- = u_{ij}\mathscr{G}_j^-, \qquad \widehat{\mathscr{G}}_i^+ = u_{ij}^*\mathscr{G}_j^+, \tag{42}$$

where the second equation follows from the first by hermitian conjugation. Requiring that $\widehat{\mathscr{G}}_i^\pm$ satisfy the same $\mathscr{N}=4$ relations as $\mathscr{G}_i^\pm$ implies that u_{ij} are SU(2) parameters: $u_{11} = u_{22}^* \equiv u_1$ and $u_{21}^* = -u_{12} \equiv u_2$ with $|u_1|^2 + |u_2|^2 = 1$. This shows that the $\mathscr{N}=4$ algebra has an SU(2) automorphism group that rotates the fermionic generators among each other. The u_i's parameterize the different embed-

dings of the $\mathscr{N} = 2$ subalgebras into the $\mathscr{N} = 4$ algebra. More explicitly, we have

$$\begin{aligned} \widehat{\widetilde{\mathscr{G}}}^+ &= \widehat{\mathscr{G}}_2^+ = u_1 \tilde{\mathscr{G}}^+ + u_2 \mathscr{G}^+, \\ \widehat{\mathscr{G}}^- &= \widehat{\mathscr{G}}_1^- = u_1 \mathscr{G}^- - u_2 \tilde{\mathscr{G}}^-, \end{aligned} \tag{43}$$

and analogous expressions for $\widehat{\mathscr{G}}^+ = \mathscr{G}_1^+$ and $\widehat{\widetilde{\mathscr{G}}}^- = \widehat{\mathscr{G}}_2^-$, which involve the complex conjugate parameters u_i^*.

It is advantageous to formulate the physical state conditions for general embeddings. This generalization also plays a role in the definition of scattering amplitudes. As will become clearer in Sect. 3, the choice of a specific embedding is related to working in a specific picture in the RNS setting. Vertex operators are therefore defined in terms of the cohomologies of the operators $\oint \widehat{\mathscr{G}}^+$ and $\oint \widehat{\widetilde{\mathscr{G}}}^+$ as in (35) and (38). Correspondingly, integrated vertex operators have zero total U(1)-charge and can be written in the form

$$\mathscr{U} = \int d^2z |\widehat{\mathscr{G}}^- \widehat{\mathscr{G}}^+|^2 \mathscr{V}. \tag{44}$$

We have $\int d^2z |\widehat{\mathscr{G}}^- \widehat{\mathscr{G}}^+|^2 \mathscr{V} = \int d^2z |\widehat{\mathscr{G}}^+ \widehat{\mathscr{G}}^-|^2 \mathscr{V}$ where one drops a total derivative under the integral. Further, if $\mathscr{V}$ is an SU(2)-singlet one has $\int d^2z |\widehat{\mathscr{G}}^- \widehat{\mathscr{G}}^+|^2 \mathscr{V} = \int d^2z |\widehat{\widetilde{\mathscr{G}}}^- \widehat{\widetilde{\mathscr{G}}}^+|^2 \mathscr{V}$. Therefore, as will be used later, $\widehat{\mathscr{G}}^+ \mathscr{U} = \widehat{\widetilde{\mathscr{G}}}^+ \mathscr{U} = 0$.

2.5 Massless Vertex Operators

Of particular interest are the universal, compactification independent vertex operators contained in the real superfield $\mathscr{V} = \mathscr{V}(x, \theta_L, \bar{\theta}_L, \theta_R, \bar{\theta}_R)$ which was discussed in [11] (cf. Appendix C for some details). It contains the degrees of freedom of $\mathscr{N} = 2$ supergravity and those of the universal tensor multiplet. It satisfies the $\mathscr{N} = 2$ primarity constraints which imply transversality constraints and linearized equations of motion for the component fields. In the amplitude computations of the next section, we will pick a certain fixed term in the u_i expansion of the integrated vertex operators (44), namely $\int |\mathscr{G}^+ \mathscr{G}^-|^2 \mathscr{V} = \int |\widetilde{\mathscr{G}}^+ \widetilde{\mathscr{G}}^-|^2 \mathscr{V}$. These operators satisfy the same properties listed below (44) as the full u_i-dependent operators (44). For this choice, the corresponding integrated vertex operator is obtained from the definition (40) and is (up to an overall numerical factor, cf. Appendix A.3)

$$\begin{aligned} \mathscr{U} = \int d^2z \Big| & \bar{d}_{\dot{\alpha}} D^2 \bar{D}^{\dot{\alpha}} - d^\alpha \bar{D}^2 D_\alpha \\ & -2i \Pi_{\alpha\dot{\alpha}} [D^\alpha, \bar{D}^{\dot{\alpha}}] + 8(\bar{\Pi}_{\dot{\alpha}} \bar{D}^{\dot{\alpha}} - \Pi^\alpha D_\alpha) \Big|^2 \mathscr{V}(z, \bar{z}). \end{aligned} \tag{45}$$

The integrated vertex operator contains (among other parts) the field strengths of the supergravity and universal tensor multiplets:

$$\int d^2z(d_L^\alpha d_R^\beta P_{\alpha\beta} + d_L^\alpha \bar{d}_R^{\dot\beta} Q_{\alpha\dot\beta}) + \text{h.c.}, \tag{46}$$

where $P_{\alpha\beta} = (\bar{D}^2 D_\alpha)_L (\bar{D}^2 D_\beta)_R \mathscr{V}$ and $Q_{\alpha\dot\beta} = (\bar{D}^2 D_\alpha)_L (D^2 \bar{D}_{\dot\alpha})_R \mathscr{V}$ are chiral and twisted-chiral superfields[7]. As discussed below, on-shell, these superfields describe the linearized Weyl multiplet and the derivative of the linearized field-strength multiplet of the universal tensor. For later purposes we also introduce $\mathscr{U}'$ and $\mathscr{U}''$ defined by $\mathscr{U} = |\mathscr{G}^+|^2 \mathscr{U}'$ and $\mathscr{U} = |\widetilde{\mathscr{G}}^+|^2 \mathscr{U}''$, i.e., $\mathscr{U}' = \int d^2z |e^\rho d^\alpha D_\alpha|^2 \mathscr{V}$ and $\mathscr{U}'' = \int d^2z |e^{-2\rho - \int J_C} \bar{d}^{\dot\alpha} \bar{D}_{\dot\alpha}|^2 \mathscr{V}$.

The complex structure moduli are in one-to-one correspondence to elements of $H^{2,1}(CY)$ and related to primary fields Ω_c of the chiral (c,c) ring [25]. The corresponding type IIB hybrid vertex operators are[8]

$$\mathscr{V}_{cc} = |e^\rho \bar\theta^2|^2 M_c \Omega_c, \qquad \mathscr{V}_{aa} = (\mathscr{V}_{cc})^\dagger = |e^{-\rho}\theta^2|^2 \bar{M}_c \bar{\Omega}_c, \tag{47}$$

where M_c is a real chiral superfield (vector multiplet). Note that in the (twisted) type IIB theory Ω_c has conformal weight $h_L = h_R = 0$, while $\bar\Omega_c$ has conformal weight $h_L = h_R = 1$. The complexified Kähler moduli are in one-to-one correspondence to elements of $H^{1,1}(CY)$ and related to primary fields Ω_{tc} of the twisted-chiral ring (c,a):

$$\mathscr{V}_{ca} = e^{\rho_L - \rho_R} \bar\theta_L^2 \theta_R^2 M_{tc} \Omega_{tc}, \qquad \mathscr{V}_{ac} = (\mathscr{V}_{ca})^\dagger = e^{-\rho_L + \rho_R} \theta_L^2 \bar\theta_R^2 \bar{M}_{tc} \bar{\Omega}_{tc}, \tag{48}$$

where M_{tc} are real twisted-chiral superfields (tensor multiplets). The conformal weight of Ω_{tc} is $h_L = 0$ and $h_R = 1$. The integrated vertex operators are

$$\begin{aligned} \mathscr{U}_{cc} &= \int d^2z M_c |G_C^-|^2 \Omega_c + \cdots, \\ \mathscr{U}_{ca} &= \int d^2z M_{tc} (G_C^-)_L (G_C^+)_R \Omega_{tc} + \cdots, \end{aligned} \tag{49}$$

where we have suppressed terms involving derivatives acting on M_c and M_{tc}. These terms carry nonzero ρ-charge and will not play a role in the discussion of the amplitudes in Sect. 4.

The vertex operators of IIA associated to elements of the (c,c) (complex structure) and (c,a) ring (Kähler) are

$$V_{cc} = e^{\rho_L - \rho_R} \bar\theta_L^2 \theta_R^2 M_{tc} \Omega_c, \qquad V_{ca} = |e^\rho \bar\theta^2|^2 M_c \Omega_{tc}. \tag{50}$$

For type IIA the conformal weights of Ω_c are $h_L = 0$ and $h_R = 1$ while Ω_{tc} has weight $h_L = h_R = 0$. The integrated vertex operators involve

[7] See Appendix C.3 for details.

[8] We are suppressing the indices distinguishing between the different elements of the ring.

$$U_{cc} = \int d^2z M_{tc}(G_C^-)_L(G_C^-)_R\Omega_c + \cdots ,$$
$$U_{ca} = \int d^2z M_c(G_C^-)_L(G_C^+)_R\Omega_{tc} + \cdots . \tag{51}$$

3 Amplitudes and Correlation Functions

In this section we review the definition of scattering amplitudes on Riemann surfaces Σ_g with genus $g \geq 2$ as given in [12]. We also collect correlation functions for chiral bosons.

3.1 Amplitudes

Scattering amplitudes of hybrid string theory are defined in [12] for $g \geq 2$ as[9]

$$F_g(u_L, u_R) = \int_{\mathscr{M}} \frac{[dm_g]}{\det(\mathrm{Im}\tau)} \times \prod_{i=1}^{g} \Big\langle \int d^2v_i \prod_{j=1}^{g-1} |\widehat{\widetilde{\mathscr{G}}}^+(v_j)|^2 |\mathscr{J}(v_g)|^2 \prod_{k=1}^{3g-3} |(\mu_k, \widehat{\mathscr{G}}^-)|^2 \prod_{l=1}^{N} \mathscr{U}_l \Big\rangle. \tag{52}$$

Since $F_g(u_L, u_R)$ is a homogeneous polynomial in both u_{iL} and u_{iR} of degree $4g-4$ (we are taking U to carry no $u_{iL,R}$ dependence as is explained in Sect. 2.4) this definitions provides a whole set of amplitudes $F_g^{n,m}$ given by the coefficients in the $u_{iL,R}$-expansion:

$$F_g(u_L, u_R) = \sum_{n,m} \binom{4g-4}{2g-2-n} \binom{4g-4}{2g-2-m} \times F_g^{n,m} u_{1L}^{2g-2+n} u_{2L}^{2g-2-n} u_{1R}^{2g-2+m} u_{2R}^{2g-2-m}, \tag{53}$$

where $2-2g \leq m, n \leq 2g-2$. We focus on either the left- or right-moving sector in the following. In view of (43) it is clear that F_g^n involves $2g-2+n$ insertions of $\widetilde{\mathscr{G}}^+$ and $\mathscr{G}^-$ and $2g-2-n$ insertions of $\mathscr{G}^+$ and $\widetilde{\mathscr{G}}^+$. It is shown in [12] that up to contact terms all distributions of $\widetilde{\mathscr{G}}^+$'s, $\mathscr{G}^-$'s, $\mathscr{G}^+$'s, and $\widetilde{\mathscr{G}}^+$'s satisfying these constraints are equivalent. We can therefore determine $F_g^{n,m}$ (53) by evaluating a single amplitude with an admissible distribution of insertions.

[9] This differs by the factor $(\det(\mathrm{Im}\tau))^{-1}$ from the expression given in [12] and [14]. We will comment on this below.

In addition there is a selection rule that relies on the cancellation of the R-parity anomaly [12]. The R-charge is

$$R = \oint \left(\partial\rho + \frac{1}{2}\theta^\alpha d_\alpha - \frac{1}{2}\bar{\theta}_{\dot{\alpha}} \bar{d}^{\dot{\alpha}} \right), \tag{54}$$

with background charge $1-g$. In the RNS formulation R coincides with the superconformal ghost-number (picture) operator, i.e., $R = \oint \mathscr{P}$. $\widetilde{\mathscr{G}}^{\pm}$ carry R-charges ∓ 1 while those of $\mathscr{G}^{\pm}$ are zero. The contribution to the R-charge of the insertions is $g-1-n$. The anomaly is therefore canceled only if the vertex operators insertions have total R-charge n. Put differently: given vertex operators $\prod_{i=1}^{N} \mathscr{U}_i$ with total R-charge n, the only non-vanishing contribution to (53) is F_g^n. This selection rule is completely analogous to the one that relies on picture charge in the RNS formulation.

It is convenient to rewrite (52) in the form

$$\begin{aligned} &F_g(u_L, u_R) \\ &\quad = \int_{\mathscr{M}} \frac{[dm_g]}{\det(\mathrm{Im}\tau)} \\ &\qquad \times \prod_{i=1}^{g} \left\langle \int d^2 v_i \prod_{j=1}^{g} |\widehat{\widetilde{\mathscr{G}}}^{+}(v_j)|^2 \prod_{k=1}^{3g-4} |(\mu_k, \widehat{\mathscr{G}}^{-})|^2 |(\mu_{3g-3}, \mathscr{J}^{--})|^2 \prod_{l=1}^{N} \mathscr{U}_l \right\rangle. \end{aligned} \tag{55}$$

This is obtained from (52) by contour deformation using $\widehat{\mathscr{G}}^{-} = \oint \widehat{\widetilde{\mathscr{G}}}^{+} \mathscr{J}^{--}$ and $\widehat{\widetilde{\mathscr{G}}}^{+} = -\oint \widetilde{\mathscr{G}}^{+} \mathscr{J}$ and the fact that $\oint \widetilde{\mathscr{G}}^{+}$ has no non-trivial OPE with any of the other insertions except a simple pole with $\mathscr{J}$. Consider the integrand of (55). As a function of, say, v_1, it has a pole only at the insertion point of $\mathscr{J}^{--}$. But the residue $\langle \prod_{i=2}^{g} \widehat{\widetilde{\mathscr{G}}}^{+}(v_i) \prod_{j=1}^{3g-3} (\mu_j, \mathscr{G}^{-}) \prod_l \mathscr{U}_l \rangle$ vanishes: each of the remaining $\widehat{\widetilde{\mathscr{G}}}^{+}(v_i)$ can be written as $-\oint \widehat{\widetilde{\mathscr{G}}}^{+} \mathscr{J}(v_i)$ and $\widehat{\widetilde{\mathscr{G}}}^{+}$ has no singular OPE with any of the other insertions. Analyticity and the fact that $\widehat{\widetilde{\mathscr{G}}}^{+}$ are Grassmann odd and of weight one, fixes the v-dependence of the integrand as $\det(\omega_i(v_j))$. The ω_i are the g holomorphic one-forms on Σ_g. In (55) we can thus replace

$$\prod \widehat{\widetilde{\mathscr{G}}}^{+}(v_i) = \det(\omega_i(v_j)) \frac{\prod \widehat{\widetilde{\mathscr{G}}}^{+}(\tilde{v}_l)}{\det(\omega_k(\tilde{v}_l))}, \tag{56}$$

where $\tilde{v}_k$ are g arbitrary points on Σ_g that can be chosen for convenience. Combining left- and right-movers the v-integrations can be performed with the result

$$\prod_{i=1}^{g} \int d^2 v_i |\det(\omega_k(v_l))|^2 \propto \det(\mathrm{Im}\tau). \tag{57}$$

τ is the period matrix of Σ_g. Using similar arguments one can rewrite

$$\frac{1}{\det(\mathrm{Im}\tau)}\Big(\int_{\Sigma_g}|\widetilde{\mathscr{G}}^{+}|^2\Big)^g \propto \Big|\prod_{i=1}^{g}\oint_{a_i}\widetilde{\mathscr{G}}^{+}\Big|^2. \tag{58}$$

The reason for the insertion $\oint\widetilde{\mathscr{G}}^{+}$ on every a-cycle of Σ_g was presented in [12, 14]: it projects to the reduced Hilbert space formed by the physical fields of an $\mathscr{N}=2$ twisted theory. Amplitudes for these states can be calculated using the rules of $\mathscr{N}=2$ topological strings.

3.2 Correlation Functions of Chiral Bosons

In this section we provide the correlation functions which are necessary to compute the amplitudes, cf. [31–33, 22, 17]. In the hybrid formulation there is no sum over spin structures and no need for a GSO projection. The correlation functions are with periodic boundary conditions around all homology cycles of the Riemann surface Σ_g.

We start with the correlators of the chiral boson H:

$$\Big\langle\prod_k e^{i\frac{q_k}{\sqrt{3}}H(z_k)}\Big\rangle = Z_1^{-1/2}F\Big(\frac{1}{\sqrt{3}}\sum q_k z_k - Q_H\Delta\Big)\prod_{i<j}E(z_i,z_j)^{\frac{1}{3}q_iq_j}\prod_l\sigma(z_l)^{\frac{1}{\sqrt{3}}Q_Hq_l}, \tag{59}$$

where Z_1 is the chiral determinant of [31–33]. The prime forms $E(z,w)$ express the pole and zero structure of the correlation function while the σ's express the coupling to the background charge. Of the remaining part F, which is due to the zero-modes of H, only the combination in which the insertion points enter will be relevant. It is, in fact, an appropriately defined theta-function [4]. Also $F(-z)=F(z)$. In the above expression (and below), z either means a point on Σ_g or its image under the Jacobi map, i.e., $\mathbf{I}(z)=\int_{p_0}^{z}\boldsymbol{\omega}$, depending on the context.

The ρ-correlation functions are subtle. The field ρ is very much like the chiral boson φ which appears in the 'Bosonization' of the superconformal (β,γ) ghost system in the RNS formulation, the only difference being the value of its background charge. In the RNS superconformal ghost system φ is accompanied by a fermionic spin 1 (η,ξ) system. Expressions for correlation functions of products of $e^{q_i\varphi(z_i)}$ which are used in RNS amplitude calculations are always done in the context of the complete (β,γ) ghost system. Following [12] our strategy will be to combine an auxiliary fermionic spin 1 (η,ξ) system with the ρ-scalar to build a bona-fide spin 1 (β,γ) system. We then compute correlation functions as in the RNS formulation, which we divide by the contribution of the auxiliary (η,ξ)-system. Following [17], we obtain

$$\left\langle \prod_k e^{q_k \rho(z_k)} \right\rangle_{(\beta,\gamma)} = \frac{Z_1^{1/2}}{\theta(\sum q_k z_k - Q_\rho \Delta)} \prod_{k<l} E(z_k, z_l)^{-q_k q_l} \prod_r \sigma(z_r)^{-Q_\rho q_r} \quad (60)$$

with $Q_\rho = -1$. As in [17], the correlation function had to be regularized due to the fact that the zero-mode contribution of the ρ-field diverges. The regularization involved a projection of the ρ-momentum plus the momentum of the regulating (η, ξ) system in the loops to arbitrary but fixed values. These projections were accompanied by factors $\oint_{a_i} \eta$ for each a-cycle on Σ and one factor of ξ to absorb its (constant) zero mode. The contribution of (η, ξ) has to be divided out in order to obtain the regulated correlators of the ρ-system. This means that (60) must be divided by

$$\left\langle \prod_{i=1}^{g} \oint_{a_i} \frac{dz_i}{2\pi i} \eta(z_i) \xi(w) \right\rangle = Z_1. \quad (61)$$

Altogether we thus find

$$\left\langle \prod_k e^{q_k \rho(z_k)} \right\rangle_{\text{reg.}} = \frac{Z_1^{-1/2}}{\theta(\sum q_k z_k + \Delta)} \prod_{k<l} E(z_k, z_l)^{-q_k q_l} \prod_r \sigma(z_r)^{q_r}. \quad (62)$$

A useful identity is the 'Bosonization formula' [31–33]:

$$\prod_{i=1}^{g} E(z_i, w) \sigma(w) = \frac{\prod_{i<j} E(z_i, z_j) \prod_{i=1}^{g} \sigma(z_i)}{Z_1^{3/2} \det(\omega_i(z_j))} \theta\left(\sum_{i=1}^{g} z_i - w - \Delta \right). \quad (63)$$

Using this identity one finds

$$\left\langle \prod_{k=1}^{g} e^{-\rho(z_k)} e^{\rho(w)} \right\rangle_{\text{reg.}} = \frac{1}{Z_1^2 \det(\omega_k(z_l))}, \quad (64)$$

which differs by a factor of $\det(\text{Im}\tau)$ from the corresponding expression used in [12].

4 Topological Amplitudes

4.1 Generalities

The expressions for F_g^n that one obtains by inserting the generators (43) into (52) in general are very involved. Certain restrictions are imposed by background charge cancellation. Since the total U(1) charge of the vertex operators is zero the insertions of $\widehat{\mathscr{G}^+}$ and $\widehat{\mathscr{G}^-}$ in (52) are precisely such that they cancel the anomaly of the total U(1) current. It is therefore sufficient to study the constraints imposed by requiring

cancellation of the background charge of the ρ-field.[10] A consequence of this constraint is that if the vertex operators are not charged under $\partial\rho$ then $|n| \leq g-1$. For $|n| < g-1$ there are several possibilities how the various parts of the operators (43) can contribute. For $|n| = g-1$ and uncharged vertex operators there is only a single amplitude that must be considered. These cases are studied in the following. We restrict to the case with $2g$ vertex operator insertions. There are then just enough insertions of θ and p to absorb their zero modes an no nontrivial contractions occur.

4.2 *R-charge* $(g-1, g-1)$

This amplitude was computed in the RNS formalism in [4]. In this section we review the computation in the hybrid formalism of [12]. Imposing ρ and H background charge saturation (52) leads to[11]

$$\mathscr{A}_g = \int_{\mathscr{M}} [dm_g] \frac{1}{|\det(\omega_i(\tilde{v}_j))|^2} \Big\langle \Big| \prod_{j=1}^{m} e^{\rho} G_C^{++}(\tilde{v}_j) \prod_{j=m+1}^{g} e^{-\rho} \bar{d}^2(\tilde{v}_j) \times \prod_{l=1}^{m} (\mu_l, e^{-2\rho - \int J_C \bar{d}^2}) \prod_{l=m+1}^{3g-3} (\mu_l, G_C^-) \Big|^2 \mathscr{U}' \mathscr{U}^{2g-1} \Big\rangle. \tag{65}$$

We have used the fact that $\oint e^{-\rho} \bar{d}^2$, when pulled off from $\mathscr{U}'$, only gets stuck at $J(v_g)$. $0 \leq m \leq g-1$ parametrizes different ways to saturate the background charges.[12] We now use the freedom to choose $\tilde{v}_l = z_l$ for $l = 1, \ldots, g$ where z_l are the arguments of the Beltrami differentials μ_l (which are integrated over). This is possible since the OPEs which one encounters are the naive products (no poles or zeros). This gives

$$\mathscr{A}_g = \int_{\mathscr{M}} [dm_g] \int \prod_{l=1}^{g} d^2 z_l \times \frac{1}{|\det(\omega_i(z_l))|^2} \Big\langle \big|(\mu_l, e^{-\rho} G_C^- \bar{d}^2(z_l))\big|^2 \prod_{k=1}^{2g-3} \big|(\mu_k, G_C^-)\big|^2 \mathscr{U}' \mathscr{U}^{2g-1} \Big\rangle \tag{66}$$

[10] Since the J_C current is a linear combination of the $\partial\rho$ and the total U(1)-current, background charge cancellation for H is then automatic.

[11] Here and in the following we drop certain numerical factors and use the notation as explained below (43).

[12] For notational simplicity we have chosen the same m for the left- and for the right-movers.

which is independent of m.[13] Its evaluation is straightforward. One easily sees that there are just enough operator insertions to absorb the p and $\bar{p}$ zero modes. θ and $\bar{\theta}$ then also only contribute with their (constant) zero modes. The p zero modes must come from the explicit d-dependence of the vertex operator. The $(p,\theta)_L$ and $(p,\theta)_R$ correlation functions contribute a factor $|Z_1|^4(\det \mathrm{Im}\tau)^2$, where the integrals over the insertion points have already been performed. What is left is the integral over the θ zero-modes which are the Grassmann odd co-ordinates of $\mathcal{N}=2$ chiral superspace. The spinor indices arrange themselves to produce $(P_{\alpha\beta}P^{\alpha\beta})^{g-1}\times P_{\gamma\delta}D_L^\gamma D_R^\delta V$. The $(\bar{p},\bar{\theta})$ correlators give a term $|Z_1|^4|\det\omega_i(z_l)|^4$, leaving only the $\bar{\theta}$ zero-mode integrations. They can be performed using $\int(d^2\bar{\theta})_L(d^2\bar{\theta})_R\Psi = \bar{D}_L^2\bar{D}_R^2\Psi|_{\bar{\theta}_L=\bar{\theta}_R=0}$. Since $\bar{D}_{\dot{\alpha}}P_{\beta\gamma}=0$, the only effect of this is to convert $D_L^\alpha D_R^\beta V$ to $P^{\alpha\beta}$. Finally, the ρ-correlator gives, using (62) and (63), $(|Z_1|^4\mid \det\omega_i(z_l)|^2)^{-1}$. The partition function of the x^m contributes a factor $|Z_1|^{-4}(\det\mathrm{Im}\tau)^{-2}$. To the given order of spacetime derivatives, the x^m-dependence of the vertex operators is only through its zero mode. Combining arguments we obtain

$$\mathscr{A}_g = \int (d^2\theta)_L(d^2\theta)_R(P_{\alpha\beta}P^{\alpha\beta})^g\int_{\mathscr{M}}[dm_g]\Big\langle\prod_{i=1}^{3g-3}|(\mu_i,G_C^-)|^2\Big\rangle. \tag{67}$$

The last part of this expression is the string partition function of the topological B-model:

$$F_g^B = \int_{\mathscr{M}}[dm_g]\Big\langle\prod_{i=1}^{3g-3}|(\mu_i,G_C^-)|^2\Big\rangle. \tag{68}$$

To determine the dependence of F_g^B on the chiral or twisted-chiral moduli one inserts the appropriate expressions (C.9) into these correlation functions. It can be shown, using the arguments of [15], that F_g^B does not depend on perturbations induced by either (c,a) or (a,c) operators. It therefore depends only on the complex structure moduli and the amplitudes calculated are therefore vector multiplet couplings (type IIB).

4.3 R-charge $(1-g, 1-g)$

Starting from (52) and imposing ρ and H-background charge saturation, one obtains, in close analogy to (65),

[13] This shows that for this amplitude all admissible distributions of vertex operators parametrized by m indeed lead to the same result and that the only subtleties that arise from contact terms are the ones analyzed in [15, 27]. We are not aware of an argument that this is generally the case.

$$\mathscr{A}'_g = \int_{\mathscr{M}} [dm_g] \frac{1}{|\det(\omega_i(\tilde{v}_j))|^2} \Big\langle \Big| \prod_{j=1}^{m} G_C^+(\tilde{v}_j) \prod_{j=m+1}^{g} e^{2\rho + \int J_C} d^2(\tilde{v}_j) \prod_{l=1}^{m} (\mu_l, e^{\rho} d^2) \times \prod_{l=m+1}^{3g-3} (\mu_l, e^{-\rho} G_C^{--}) \Big|^2 \mathscr{U}'' \mathscr{U}^{2g-1} \Big\rangle. \tag{69}$$

$0 \le m \le g-1$ parametrizes the different ways of saturating the background charges. By appropriate choices of the $\tilde{v}_j$ this amplitude can be brought to the form

$$\mathscr{A}'_g = \int_{\mathscr{M}} [dm_g] \int \prod_{j=1}^{g} d^2 z_j \frac{1}{|\det \omega_i(z_j)|^2} \Big\langle \Big| (\mu(z_j), e^{\rho} d^2 G_C^+(z_j)) \times \prod_{k=1}^{2g-3} (\mu_k, e^{-\rho} G_C^{--}) \Big|^2 \mathscr{U}'' \mathscr{U}^{2g-1} \Big\rangle, \tag{70}$$

which shows that also this amplitude is independent of m. However, its evaluation is most easily done for a different choice of the insertion points $\tilde{v}_j$. To fix them, we start from (69) with the choice $m = 0$ and compute the ρ and the H correlators. Their product is, using (59) and (62),

$$\frac{1}{Z_1} \frac{F(\sqrt{3}\sum \tilde{v}_j - \frac{2}{\sqrt{3}} \sum z_k - \sqrt{3} w + \sqrt{3}\Delta)}{\theta(2\sum \tilde{v}_j - \sum z_k - 2w + \Delta)} \times \frac{\prod_{k<l} E(z_k, z_l)^{\frac{1}{3}} \prod_j E(\tilde{v}_j, w) \prod_k \sigma(z_k) \sigma(w)}{\prod_{i<j} E(\tilde{v}_i, \tilde{v}_j) \prod_j \sigma(\tilde{v}_j)}, \tag{71}$$

where we have only displayed the holomorphic part. With the help of the identity (63) this is equal to

$$\frac{1}{(Z_1)^{\frac{5}{2}}} \frac{F(\sqrt{3}\sum \tilde{v}_j - \frac{2}{\sqrt{3}} \sum z_k - \sqrt{3} w + \sqrt{3}\Delta)}{\theta(2\sum \tilde{v}_j - \sum z_k - 2w + \Delta)} \tag{72}$$

$$\times \frac{\theta(\sum \tilde{v}_j - w - \Delta)}{\det w_i(\tilde{v}_j)} \cdot \prod_{k<l} E(z_k, z_l)^{\frac{1}{3}} \prod_k \sigma(z_k). \tag{73}$$

We now choose the g positions $\tilde{v}_j$ such that $\mathbf{I}(\sum \tilde{v}_j - w - \Delta) = \mathbf{I}(2\sum \tilde{v}_j - \sum z_k - 2w + \Delta)$. Then the theta functions cancel and the remaining terms are

$$\frac{1}{(Z_1)^{\frac{5}{2}} \det \omega_i(\tilde{v}_j)} \cdot F\Big(\frac{1}{\sqrt{3}} \sum z_k - \sqrt{3}\Delta\Big) \cdot \prod_{k<l} E(z_k, z_l)^{\frac{1}{3}} \prod_k \sigma(z_k). \tag{74}$$

This can be written as

$$\frac{1}{Z_1^2 \det \omega_i(\tilde{v}_j)} \left\langle \prod_{k=1}^{3g-3} e^{-\frac{i}{\sqrt{3}} H(z_k)} \right\rangle. \tag{75}$$

The $p, \theta, \bar{p}$ and $\bar{\theta}$ correlators are as in the previous amplitude (with the roles on barred and unbarred variables interchanged) and one finally obtains

$$\mathscr{A}'_g = \int (d^2\bar{\theta})_L (d^2\bar{\theta})_R (\bar{P}_{\dot{\alpha}\dot{\beta}} \bar{P}^{\dot{\alpha}\dot{\beta}})^g \int_{\mathscr{M}} [dm_g] \left\langle \prod_{i=1}^{3g-3} |(\mu_i, \check{G}_C^-)|^2 \right\rangle. \tag{76}$$

Here $\check{G}_C^- = e^{-\frac{i}{\sqrt{3}} H} G'_C$ where G'_C is defined to be $G_C^+ = e^{\frac{i}{\sqrt{3}} H} G'_C$. Note that G_C^- and $\check{G}_C^-$ both have conformal weight two. The internal amplitude multiplying the spacetime part is the complex conjugate of the B-model amplitude (68): this follows from the fact that the expression (74) can be written as

$$\frac{1}{Z_1^2 \det \omega_i(\tilde{v}_j)} \left\langle \prod_{k=1}^{3g-3} e^{\frac{i}{\sqrt{3}} H(z_k)} \right\rangle_{Q_H = \sqrt{3}}, \tag{77}$$

where we used (59) but with the reversed background charge as compared to (75). This happens if one chooses the opposite twisting in (6). Since the operators $\check{G}_C^-$ and G_C^+ both contain the same operator G'_C, the internal part of the amplitude (76) is equal to

$$\left\langle \prod_{i=1}^{3g-3} |(\mu_i, \check{G}_C^-)|^2 \right\rangle_{++} = \left\langle \prod_{i=1}^{3g-3} |(\mu_i, G_C^+)|^2 \right\rangle_{--}. \tag{78}$$

The subscripts refer to the two possible twistings $T_C \to T_C + \frac{1}{2}\partial J_C$ and $T_C \to T_C - \frac{1}{2}\partial J_C$ for left- and right-movers. Finally, since for unitary theories $(G_C^-)^\dagger = G_C^+$, the right-hand side of (78) is the complex conjugate of F_g^B given in (68), and therefore $\mathscr{A}'_g$ defined in (69) is the complex conjugate of the chiral amplitude $\mathscr{A}_g$ of (65).

4.4 *R*-charges $(g-1, 1-g)$ and $(1-g, g-1)$

The 'mixed' amplitudes with R-charges $(g-1, 1-g)$ and $(1-g, g-1)$ can now be written down immediately. They are expressed as integrals over twisted chiral superspace and involve the superfields $Q_{\alpha\dot{\beta}}$ and $\bar{Q}_{\dot{\alpha}\beta}$. They are

$$\mathscr{A}''_g = \int (d^2\theta)_L (d^2\bar{\theta})_R (Q_{\alpha\dot{\beta}} Q^{\alpha\dot{\beta}})^g \int_{\mathscr{M}} [dm_g] \left\langle \prod_{i=1}^{3g-3} (\mu_i, G_C^-)_L (\bar{\mu}_i, \check{G}_C^-)_R \right\rangle + \text{c.c.} \tag{79}$$

By the same arguments as given before, one shows that this type IIB string amplitude only depends on deformations in the (a, c) (and (c, a) for the complex conjugate

piece) ring, i.e., on Kähler moduli. In type IIB, these are in tensor multiplets. From the discussion in Sect. 4.3 it also follows that

$$\int_{\mathscr{M}}[dm_g]\left\langle\prod_{i=1}^{3g-3}(\mu_i, G_C^-)_L(\bar{\mu}_i, \check{G}_C^-)_R\right\rangle_{++}$$
$$=\int_{\mathscr{M}}[dm_g]\left\langle\prod_{i=1}^{3g-3}(\mu_i, G_C^-)_L(\bar{\mu}_i, G_C^+)_R\right\rangle_{+-}=F_g^A, \tag{80}$$

which is the topological A-model amplitude.

So far we have computed amplitudes of type IIB string theory. To compute type IIA amplitudes we need to twist the left- and right-moving internal SCFTs oppositely. In the amplitudes this induces the following changes: $(G_C^-)_R \to (G_C^+)_R$ and $(\check{G}_C^-)_R \to (\check{G}_C^+)_R$ where $\check{G}_C^+ = e^{\frac{i}{\sqrt{3}}H}\bar{G}'_C$. Due to the opposite twist, the conformal weights are preserved under this operation. For instance, the spacetime part of (67) gets combined with F_g^A, that of (79) with F_g^B. According to (C.9) and (C.12), F_g^A depends on the moduli contained in vector multiplets, F_g^B on those contained in tensor multiplets.

4.5 Summary of the Amplitude Computation

We have recomputed certain chiral and twisted-chiral couplings that involve g powers of P^2 or Q^2, respectively, using hybrid string theory. The amplitudes involve the topological string partition functions F_g^A and F_g^B. F_g^A depends on the moduli parametrizing the (c, a) ring, F_g^B on those of the (c, c) ring. In type IIA or type IIB, these are contained in spacetime chiral (vector) or twisted-chiral (tensor) multiplets, as summarized in the table. The dependence on the moduli of the complex

Type IIA	Type IIB
$(P^2)^g F_g^A$ (c, a): vector	$(P^2)^g F_g^B$ (c, c): vector
$(Q^2)^g F_g^B$ (c, c): tensor	$(Q^2)^g F_g^A$ (c, a): tensor

conjugate rings is only through the holomorphic anomaly [15]. As discussed in [11, 13], on-shell, the superfield $P_{\alpha\beta}$ describes the linearization of the Weyl multiplet. Its lowest component is the selfdual part of the graviphoton field strength, $P_{\alpha\beta}| = F_{\alpha\beta}$. The $\theta_L\theta_R$-component is the selfdual part $C_{\alpha\beta\gamma\delta}$ of the Weyl tensor. The bosonic components of $Q_{\alpha\dot{\beta}}$ are $Q_{\alpha\dot{\beta}}| = \partial_{\alpha\dot{\beta}}Z$, where Z is the complex R-R-scalar of the RNS formulation of the type II string; its $\theta_L\bar{\theta}_R$-component is $\partial_{\alpha\dot{\alpha}}\partial_{\beta\dot{\beta}}S$. The real component of S is the dilaton, its imaginary component is dual to the antisymmetric tensor of the NS-NS-sector. These results can be obtained by explicit computation from the θ-expansion of the superfield V. After integrating (67) and (79) over chiral

and twisted-chiral superspace, respectively, $2g-2$ powers of $F_{\alpha\beta}$ are coupled to two powers of $C_{\alpha\beta\gamma\delta}$, while $2g-2$ powers of ∂Z are coupled to two powers of $\partial^2 S$, with the tensorial structure discussed in [4]. In [11, 8, 29] the question is addressed how these (and other) couplings can be described in an off-shell (projective) superspace description at the non-linearized level.

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A Appendix: Conventions and Notations

A.1 Spinors and Superspace

Throughout this paper we use the conventions of Wess and Bagger [34, 16]. In particular the space-time metric is $\eta^{mn} = \mathrm{diag}(-1,+1,+1,+1)$ and the spinor metric is $\epsilon^{12} = \epsilon^{\dot{1}\dot{2}} = \epsilon_{21} = \epsilon_{\dot{2}\dot{1}} = 1$. Spinor indices are raises and lowered as $\psi^\alpha = \epsilon^{\alpha\beta}\psi_\beta$, $\psi_\alpha = \epsilon_{\alpha\beta}\psi^\beta$, and likewise for the dotted indices. Spinor indices are contracted in the following way: $\psi\chi = \psi^\alpha\chi_\alpha$, $\bar\psi\bar\chi = \bar\psi_{\dot\alpha}\bar\chi^{\dot\alpha}$. Barred spinors always have dotted indices. We define $x_{\alpha\dot\alpha} = \sigma^m_{\alpha\dot\alpha}x_m$ where $\sigma^m_{\alpha\dot\alpha} = (-\mathbf{1},\boldsymbol{\sigma})$ with $v^m v_m = -\frac{1}{2}v^{\alpha\dot\alpha}v_{\alpha\dot\alpha}$ and $\partial_{\alpha\dot\alpha} = \sigma^m_{\alpha\dot\alpha}\partial_m$ such that $\partial_{\alpha\dot\alpha}x^{\beta\dot\beta} = -2\delta_\alpha^\beta\delta_{\dot\alpha}^{\dot\beta}$. Starting from the supersymmetry invariant one-forms on superspace

$$\begin{aligned} e^a &= dx^a - id\theta\sigma^a\bar\theta + i\theta\sigma^a d\bar\theta, \\ e^\alpha &= d\theta^\alpha, \\ e_{\dot\alpha} &= d\bar\theta_{\dot\alpha}, \end{aligned} \tag{A.1}$$

one finds their pullbacks to the world-sheet

$$\begin{aligned} \Pi^{\alpha\dot\alpha} &= \partial x^{\alpha\dot\alpha} + 2i\partial\theta^\alpha\bar\theta^{\dot\alpha} + 2i\partial\bar\theta^{\dot\alpha}\theta^\alpha, \\ \Pi^\alpha &= \partial\theta^\alpha, \\ \bar\Pi_{\dot\alpha} &= \partial\bar\theta_{\dot\alpha}, \end{aligned} \tag{A.2}$$

and likewise for the right-movers. Expressed in terms of the Π's, the energy momentum tensor of the x, θ, p variables is

$$T = \frac{1}{4}\Pi^{\alpha\dot\alpha}\Pi_{\alpha\dot\alpha} - \Pi^\alpha d_\alpha - \bar\Pi_{\dot\alpha}\bar d^{\dot\alpha} - \frac{1}{2}(\partial\rho)^2 + \frac{1}{2}\partial^2\rho, \tag{A.3}$$

with d_α and $\bar d^{\dot\alpha}$ defined by

$$
\begin{aligned}
d_\alpha &= p_\alpha + i\bar{\theta}^{\dot{\alpha}}\partial x_{\alpha\dot{\alpha}} - \bar{\theta}^2\partial\theta_\alpha + \frac{1}{2}\theta_\alpha\partial\bar{\theta}^2, \\
\bar{d}^{\dot{\alpha}} &= \bar{p}^{\dot{\alpha}} + i\theta_\alpha\partial x^{\alpha\dot{\alpha}} - \theta^2\partial\bar{\theta}^{\dot{\alpha}} + \frac{1}{2}\bar{\theta}^{\dot{\alpha}}\partial\theta^2.
\end{aligned}
\tag{A.4}
$$

A.2 Hybrid Variables and $\mathcal{N} = 2$ Algebra

The singular parts of the operator products of the hybrid variables are

$$
\begin{aligned}
x^m(z,\bar{z})x^n(w,\bar{w}) &\sim -\eta^{mn}\ln|z-w|^2, \\
\theta_\alpha(z)p^\beta(w) &\sim \frac{\delta_\alpha^\beta}{(z-w)}, \\
\bar{\theta}^{\dot{\alpha}}(z)\bar{p}_{\dot{\beta}}(w) &\sim \frac{\delta_{\dot{\beta}}^{\dot{\alpha}}}{(z-w)}, \\
\rho(z)\rho(w) &\sim -\ln(z-w).
\end{aligned}
\tag{A.5}
$$

Both (A.3) and (A.5) follow from the action (1). We also note that

$$
d_\alpha(z)\bar{d}_{\dot{\alpha}}(w) \sim \frac{2i\Pi_{\alpha\dot{\alpha}}(w)}{(z-w)}, \tag{A.6}
$$

while dd and $\bar{d}\bar{d}$ are finite. The action of d and $\bar{d}$ on a generic superfield M is

$$
\begin{aligned}
d_\alpha(z)M(w) &\sim -\frac{D_\alpha M(w)}{(z-w)} \quad \text{where } D_\alpha \equiv \quad \partial_\alpha + i\bar{\theta}^{\dot{\alpha}}\partial_{\alpha\dot{\alpha}} \\
d_{\dot{\alpha}}(z)M(w) &\sim -\frac{\bar{D}_{\dot{\alpha}} M(w)}{(z-w)} \quad \text{where } \bar{D}_{\dot{\alpha}} \equiv -\bar{\partial}_{\dot{\alpha}} - i\theta^\alpha\partial_{\alpha\dot{\alpha}}
\end{aligned}
\tag{A.7}
$$

with $\{D_\alpha, \bar{D}_{\dot{\alpha}}\} = -2i\partial_{\alpha\dot{\alpha}}$. For later purposes we note the useful identities

$$
[D_\alpha, \bar{D}^2] = -4i\partial_{\alpha\dot{\alpha}}\bar{D}^{\dot{\alpha}}, \qquad \frac{1}{16}[\bar{D}^2, D^2] = \partial^m\partial_m + \frac{i}{2}\partial_{\alpha\dot{\alpha}}D^\alpha\bar{D}^{\dot{\alpha}} \tag{A.8}
$$

One defines the space-time supercharges

$$
\begin{aligned}
Q_\alpha &= \oint\left(p_\alpha - i\bar{\theta}^{\dot{\alpha}}\partial x_{\alpha\dot{\alpha}} + \frac{1}{2}\bar{\theta}^2\partial\theta_\alpha\right) \\
\bar{Q}^{\dot{\alpha}} &= \oint\left(\bar{p}^{\dot{\alpha}} - i\theta_\alpha\partial x^{\alpha\dot{\alpha}} + \frac{1}{2}\theta^2\partial\bar{\theta}^{\dot{\alpha}}\right)
\end{aligned}
\tag{A.9}
$$

such as to satisfy

$$\begin{aligned}\{Q_\alpha, \bar{Q}_{\dot\alpha}\} &= -2i \oint \partial x_{\alpha\dot\alpha} \\ \{Q_\alpha, Q_\beta\} &= \{\bar{Q}_{\dot\alpha}, \bar{Q}_{\dot\beta}\} = 0\end{aligned} \tag{A.10}$$

and to (anti)commute with the d's and Π's. In deriving these relations we have dropped total derivatives involving fermion bilinears. Note that $\{Q_\alpha, \bar{Q}_{\dot\alpha}\}\varphi = 2i\sigma^m_{\alpha\dot\alpha}\partial_m\varphi$, as expected.

Vertex operators for physical states are required to be primary. By definition, a primary state is annihilated by all positive modes of the generators of the superconformal algebra. For a superfield $\mathscr{U}$ which is independent of ρ and of the internal CFT this leads to the on-shell conditions $\partial_m\partial^m\mathscr{U} = D^2\mathscr{U} = \bar{D}^2\mathscr{U} = 0$.

A.3 The Integrated Vertex Operator

We compute [19, 20]

$$\mathscr{W}(z) = G^-G^+\mathscr{V}(z) \tag{A.11}$$

where $\mathscr{V}(z)$ is primary (assumed to be bosonic) and depends on $x, \theta, \bar\theta$ but is independent of ρ. The first commutator is straightforward to compute. With the help of (A.7) one finds

$$\sqrt{32}G^+\mathscr{V}(w) = \oint_{C_w} dz e^{-\rho(z)}\left(-\frac{\bar{D}^2\mathscr{V}(w)}{(z-w)^2} + \frac{2\bar{d}\bar{D}\mathscr{V}(w)}{z-w}\right) = 2e^{-\rho(w)}\bar{d}_{\dot\alpha}\bar{D}^{\dot\alpha}\mathscr{V}(w) \tag{A.12}$$

where $\bar{D}^2\mathscr{V} = 0$ has been used. The computation of the second commutator is more involved. Applying the rules stated in [21] one finds

$$\begin{aligned}&-32G^-G^+\mathscr{V}(w) \\ &\quad= 16\partial\bar\theta_{\dot\alpha}\bar{D}^{\dot\alpha}\Phi(w) + 8id^\alpha\partial_{\alpha\dot\alpha}\bar{D}^{\dot\alpha}\mathscr{V}(w) \\ &\qquad- 4i\Pi_{\alpha\dot\alpha}D^\alpha\bar{D}^{\dot\alpha}\mathscr{V}(w) + \bar{d}_{\dot\alpha}D^2\bar{D}^{\dot\alpha}\mathscr{V}(w)\end{aligned} \tag{A.13}$$

where normal ordering is implied in all terms. A term $-4i\partial\rho\partial_{\alpha\dot\alpha}D^\alpha\bar{D}^{\dot\alpha}\mathscr{V}(w)$ has been dropped; using (A.8) it can be shown to vanish if $\mathscr{V}$ is primary, as we have assumed. One can cast (A.13) into a more symmetric form if one adds a total derivative[14] of $\mathscr{V}$:

$$\begin{aligned}&-32G^-G^+\mathscr{V}(w) + 8\partial\mathscr{V}(w) \\ &\quad= -8(\Pi^\alpha D_\alpha - \bar\Pi_{\dot\alpha}\bar{D}^{\dot\alpha})\mathscr{V}(w) - 2i\Pi_{\alpha\dot\alpha}[D^\alpha, \bar{D}^{\dot\alpha}]\mathscr{V}(w) \\ &\qquad+ (\bar{d}_{\dot\alpha}D^2\bar{D}^{\dot\alpha} - d^\alpha\bar{D}^2D_\alpha)\mathscr{V}(w).\end{aligned} \tag{A.14}$$

Here we have used the notation defined in (A.2).

[14] This total derivative could contribute to boundary terms when two vertex operators collide and might thus play an important role in amplitude computation.

B Appendix: Mapping the RNS to the Hybrid Variables

In this appendix we give the details of the field mapping suppressed in Sect. 2.3 which relate the RNS and the hybrid variables, following closely [9]. It is easiest to split this map into a part involving a field redefinition and one involving a similarity transformation. The field redefinition defines a set of Green-Schwarz-like variables in terms of the RNS variables. These are then related to the hybrid variables by a similarity transformation.

B.1 Field Redefinition from RNS to Chiral GS Variables

From the RNS variables one first forms a set of variables according to (18) and (25). Following [7, 12], these are called the "chiral GS-variables". In [7, 12] these variables were denoted collectively by $\tilde{\Phi}$, whereas in [9] they were labeled with the superscript "old". In this section we label the chiral GS-variables with the subscript "GS" for clarity, while this is suppressed in the main text.

In order to achieve the correct normalization (29) we must perform the following rescaling of RNS variables:

$$\begin{aligned} &b \to 2\sqrt{2}b, && c \to (2\sqrt{2})^{-1}c, && \eta \to 2\sqrt{2}\eta, \\ &\xi \to (2\sqrt{2})^{-1}\xi, && e^{-\varphi} \to 2\sqrt{2}e^{-\varphi}. \end{aligned} \tag{B.1}$$

These rescalings preserve all the OPEs. We use the rescaled RNS variables in this section.

B.2 Similarity Transformation Relating Chiral GS to Hybrid Variables

The chiral GS-variables Φ_{GS}, including those of the internal SCFT, are related to the hybrid ones Φ by the similarity transformation

$$(\Phi)_{\mathrm{GS}} = e^{\mathscr{M}+\mathscr{M}_C^-}(\Phi)e^{-(\mathscr{M}+\mathscr{M}_C^-)}. \tag{B.2}$$

We have defined

$$\mathscr{M} = \oint i\theta^\alpha\bar{\theta}^{\dot{\alpha}}\partial x_{\alpha\dot{\alpha}} + \frac{1}{4}(\theta^2\partial\bar{\theta}^2 - \bar{\theta}^2\partial\theta^2), \tag{B.3}$$

and

$$\mathscr{M}_C^- = -\sqrt{2}c_- \oint e^{-\rho}\theta^2 G_C^-, \qquad \mathscr{M}_C^+ = \sqrt{2}c_+ \oint e^{\rho}\bar{\theta}^2 G_C^+, \tag{B.4}$$

with $[\mathscr{M}_C^{\pm}, \mathscr{M}] = 0$. One way to see that this is indeed the correct transformation is to verify that

$$e^{\mathscr{M}}\, p_\alpha e^{-\mathscr{M}} = d_\alpha, \tag{B.5}$$

from which

$$e^{\mathscr{M}+\mathscr{M}_C^-}\left(\frac{1}{\sqrt{32}} e^{\rho}\, p^\alpha\, p_\alpha\right) e^{-(\mathscr{M}+\mathscr{M}_C^-)} = \frac{1}{\sqrt{32}} e^{\rho} d^\alpha d_\alpha + c_- G_C^- = \mathscr{G}^- \tag{B.6}$$

follows. By definition (B.2), the l.h.s. of this expression equals $(\frac{1}{\sqrt{32}} e^{-\rho}\, p^\alpha\, p_\alpha)_{\mathrm{GS}}$, which, according to (18) and (B.1), equals the RNS ghost field b. One therefore concludes

$$b = \left(\frac{1}{\sqrt{32}} e^{-\rho}\, p^\alpha\, p_\alpha\right)_{\mathrm{GS}} = \frac{1}{\sqrt{32}} e^{-\rho} d^\alpha d_\alpha + c_- G_C^- = \mathscr{G}^- \tag{B.7}$$

as stated in (26).

It can be verified that for the generators $\mathscr{J} = \mathscr{J}_{\mathrm{GS}}$, $\mathscr{T} = \mathscr{T}_{\mathrm{GS}}$, $\mathscr{J}^{\pm\pm} = \mathscr{J}_{\mathrm{GS}}^{\pm\pm}$. They are therefore not affected by (B.2). These results were used in Sect. 2.4.

B.3 Hermitian Conjugation of the Hybrid Variables

Hermitian conjugation acts on the hybrid variables as

$$(x^m)^\dagger = x^m, \qquad (\theta^\alpha)^\dagger = \bar{\theta}^{\dot{\alpha}}, \qquad (p_\alpha)^\dagger = -\bar{p}_{\dot{\alpha}}. \tag{B.8}$$

From these properties one concludes that $(\partial x^m)^\dagger = -\partial x^m$ and $(\partial\theta^\alpha)^\dagger = -\partial\bar{\theta}^{\dot{\alpha}}$. In addition, we define

$$\rho^\dagger = -\rho - \ln z + i\pi, \qquad H^\dagger = H - i\sqrt{3}\ln z + \pi\sqrt{3}. \tag{B.9}$$

Some comments are in order here. The $\ln z$ terms are due to the background charges of currents $J = \partial\rho$ and $J_C = i\sqrt{3}\partial H$. In the presence of a (real) background charge Q, the operator product of the energy-momentum tensor and a generic (hermitian) current is modified to $T(z)\,j(w) \sim \frac{Q}{(z-w)^3} + \frac{j(w)}{(z-w)^2} + \frac{\partial j(w)}{(z-w)}$. In terms of the modes this reads $[L_n, j_m] = \frac{1}{2}Qn(n+1)\delta_{n+m} - m j_{n+m}$ and implies $j_n^\dagger = j_{-n} - Q\delta_{n,0}$ and $L_n^\dagger = L_{-n} - Q(n-1)j_{-n}$. These results are to be applied for the currents $j = -\partial\rho = -J$ and $j = J_C$ with the background charges -1 and -3, respectively. This implies that $(p_\rho)^\dagger = p_\rho - 1$ and $(p_H)^\dagger = p_H + \sqrt{3}$ such that the cocycle factors introduced in Sect. 2.1 satisfy $(c_+)^\dagger = c_-$. The constant shifts $+i\pi$ and $+\pi\sqrt{3}$ seem to be needed in order to obtain the correct hermiticity relations between various $\mathscr{N} = 4$ generators and the correct algebra. It is consistent with the fact that ρ and H are compact bosons with periodicity $2\pi i$ and $2\pi\sqrt{3}$, respectively. Using the general CFT rule, $[\varphi(z)]^\dagger = \varphi^\dagger(\frac{1}{\bar{z}})\bar{z}^{-2h}$, valid for a primary field φ of dimension

h, one shows $\exp(q\rho)^\dagger = (-1)^q \exp(-q\rho)$ and $\exp(\frac{iq}{\sqrt{3}H})^\dagger = (-1)^q \exp(-\frac{iq}{\sqrt{3}}H)$. This, together with $(G_C^\pm)^\dagger = G_C^\mp$, completes the discussion of hermitian conjugation of the hybrid variables.

B.4 Hermitian Conjugation of the RNS Variables

Going through the sequence of similarity transformations and field redefinitions outlined in Appendices B.1 and B.2, the hybrid conjugation rules induce a hermitian conjugation for the RNS variables. This conjugation is not the standard one. We discuss this in detail below and obtain, as a side-product, the a justification for the complete dictionary given in (29).

Using $\mathscr{M}^\dagger = \mathscr{M}$ and $(\mathscr{M}_C^-)^\dagger = \mathscr{M}_C^+$, hermitian conjugation of (B.6) and (B.7) (or direct computation) yields

$$\begin{aligned} b^\dagger &= e^{-(\mathscr{M}+\mathscr{M}_C^+)} \left(-\frac{1}{\sqrt{32}} e^{-\rho}\, \bar{p}_{\dot\alpha} \bar{p}^{\dot\alpha}\right) e^{\mathscr{M}+\mathscr{M}_C^+} \\ &= -\frac{1}{\sqrt{32}} e^{-\rho} \bar{d}_{\dot\alpha} \bar{d}^{\dot\alpha} - c_+ G_C^+ = \mathscr{G}^+. \end{aligned} \tag{B.10}$$

As is argued below, this expression equals the current j_{BRST} in accordance with (26). The hybrid hermiticity properties therefore imply in particular that $b^\dagger = j_{\mathrm{BRST}}$. We work this out in more detail: one first remarks that (B.10) is not the similarity transformation (B.2), since latter involves the charge $\mathscr{M} + \mathscr{M}_C^-$. In fact, under this transformation $-\frac{1}{\sqrt{32}} e^{-\rho}\, \bar{p}^2$ is mapped to

$$\begin{aligned} e^{\mathscr{M}+\mathscr{M}_C^-} \left(-\frac{1}{\sqrt{32}} e^{-\rho}\, \bar{p}_{\dot\alpha} \bar{p}^{\dot\alpha}\right) e^{-(\mathscr{M}+\mathscr{M}_C^-)} &= \left(-\frac{1}{\sqrt{32}} e^{-\rho}\, \bar{p}_{\dot\alpha} \bar{p}^{\dot\alpha}\right)_{\mathrm{GS}} \\ &= -b\gamma^2. \end{aligned} \tag{B.11}$$

The first equality is just the definition (B.2), while the second one is a consequence of the field redefinition (18) and (B.1). Inverting this relation and inserting the result in (B.10) one finds

$$b^\dagger = e^{-\mathscr{R}}(-b\gamma^2) e^{\mathscr{R}}. \tag{B.12}$$

The claim is that the r.h.s. is j_{BRST}. We have defined

$$e^{\mathscr{R}} = e^{\mathscr{M}+\mathscr{M}_C^-} e^{\mathscr{M}+\mathscr{M}_C^+} = e^{2\mathscr{M}+\mathscr{M}_C^-+\mathscr{M}_C^++\frac{1}{2}[\mathscr{M}_C^-,\mathscr{M}_C^+]}. \tag{B.13}$$

While the first equality is the definition, the second one holds whenever one has $[\mathscr{M}_C^-, [\mathscr{M}_C^-, \mathscr{M}_C^+]] = [\mathscr{M}_C^+, [\mathscr{M}_C^+, \mathscr{M}_C^-]] = 0$. That this is indeed the case as can be seen by calculating the commutator

$$[\mathscr{M}_C^-, \mathscr{M}_C^+] = 2 \oint \left[\theta^2 \bar{\theta}^2 \left(J_C + \frac{c}{3} \partial \rho \right) - \frac{c}{3} \bar{\theta}^2 \partial \theta^2 \right]. \tag{B.14}$$

We used the normalization

$$G_C^-(z) G_C^+(w) \sim \frac{\frac{c}{3}}{(z-w)^3} - \frac{J_C(w)}{(z-w)^2} + \frac{T_C(w) - \partial J_C(w)}{z-w}, \tag{B.15}$$

which follows from (5). Since $G_C^\pm$ has only a simple pole with J_C, $\mathscr{M}_C^\pm$ commute with this commutator and (B.13) is established. The explicit expression for $\mathscr{R}$ in terms of hybrid variables is

$$\begin{aligned} \mathscr{R} = \oint \Big[& 2i \theta^\alpha \bar{\theta}^{\dot{\alpha}} \partial x_{\alpha \dot{\alpha}} - \sqrt{2} c_- e^{-\rho} \theta^2 G_C^- + \sqrt{2} c_+ e^{\rho} \bar{\theta}^2 G_C^+ \\ & + \theta^2 \bar{\theta}^2 \left(J_C + \frac{c}{3} \partial \rho \right) + \left(1 + \frac{c}{3} \right) \theta^2 \partial \bar{\theta}^2 \Big]. \end{aligned} \tag{B.16}$$

In order to evaluate the r.h.s. of (B.12), we re-express this operator in terms of RNS variables. Thereby one must bear in mind that the field map (B.2) affects all fields, including the generators of the internal SCFT. In particular, one finds that under (B.2)

$$\begin{aligned} (\partial x_{\alpha \dot{\alpha}})_{\mathrm{GS}} &= \partial x_{\alpha \dot{\alpha}} + 2i \partial (\theta_\alpha \bar{\theta}_{\dot{\alpha}}), \\ (c_+ e^{\rho} \bar{\theta}^2 G_C^+)_{\mathrm{GS}} &= c_+ e^{\rho} \bar{\theta}^2 G_C^+ + \sqrt{2} \left[\theta^2 \bar{\theta}^2 \left(J_C + \frac{c}{3} \partial \rho \right) - \frac{c}{3} \bar{\theta}^2 \partial \theta^2 \right], \end{aligned} \tag{B.17}$$

while θ^α, $\bar{\theta}_{\dot{\alpha}}$, and the combinations $\theta^2 \bar{\theta}^2 J_C$ and $\theta^2 \bar{\theta}^2 \partial \rho$ remain unaffected. Using (21), (23), and (25) and dropping total derivatives one finds that $\mathscr{R}$ is the following simple expression in RNS variables:[15]

$$\mathscr{R} = \oint \left[c \xi e^{-\varphi} T_F + \frac{1}{2} e^{-2\varphi} c \partial c \xi \partial \xi \left(\partial \varphi + \frac{c-9}{3} \partial \sigma \right) \right]. \tag{B.18}$$

The terms in (B.16) involving the current $\breve{J}_C$ have canceled and the last term in (B.18) vanishes for $c = 9$. We have defined $T_F = T_F^{x,\psi} + \breve{G}_C^+ + \breve{G}_C^-$, where $T_F^{x,\psi}$ is the supercurrent of the space-time matter sector. It is normalized as $T_F(z) T_F(w) \sim \frac{2}{3}(c^{x,\psi} + c)(z-w)^{-3} + \cdots$, with $c^{x,\psi} = 6$ [see also (B.15)].

Using the conventions of [23] one can verify that (B.12) with $\mathscr{R}$ given in (B.18) indeed produces the BRST current (this current differs from the usual current by addition of total derivative terms),

[15] In order to obtain this result, one must take special care of the overall signs for the RNS expressions of θ^2, $\bar{\theta}^2$, $\theta^2 \partial \bar{\theta}^2$, and alike. We suppress these details in this note.

$$
\begin{aligned}
e^{-\mathscr{R}}(-b\gamma^2)e^{\mathscr{R}} &= j_{\mathrm{BRST}} \\
&= c\left(T - b\partial c - \frac{1}{2}(\partial\varphi)^2 - \partial^2\varphi + \frac{1}{2}(\partial\chi)^2 + \frac{1}{2}\partial^2\chi\right) \\
&\quad + \gamma T_F - b\gamma^2 + \partial^2 c + \partial(c\partial\chi),
\end{aligned}
\tag{B.19}
$$

where $T = T^{x,\psi} + \breve{T}_C$. Details of this computation can be found in [1]. The BRST charge is

$$
Q_{\mathrm{BRST}} = \oint\left[cT + e^{\varphi}\eta T_F + bc\partial c + be^{2\varphi}\eta\partial\eta + c\left(\partial\xi\,\eta - \frac{1}{2}(\partial\varphi)^2 - \partial^2\varphi\right)\right]
$$

and coincides with the charge which follows from the BRST current in [28] after Bosonization. From this one derives an expression for the picture-changing operator in bosonized form,

$$
Z = \{Q_{\mathrm{BRST}}, \xi\} = e^{\varphi}T_F + c\partial\xi - b\partial\eta e^{2\varphi} - \partial(b\eta^2 e^{2\varphi}),
\tag{B.20}
$$

which enters in (28).

It does not seem possible to give a closed formula for the hermitian conjugation of a generic RNS field. If, however, an RNS field Φ_{RNS} is expressible in terms of chiral GS-variables, $\Phi_{\mathrm{GS}} = \Phi_{\mathrm{RNS}}$, one can use the same argument as above and deduce the rule:

$$
(\Phi_{\mathrm{RNS}})^{\dagger} = e^{-\mathscr{R}}\Psi_{\mathrm{RNS}}e^{\mathscr{R}}, \quad \text{with } \Psi_{\mathrm{RNS}} := (\Phi_{\mathrm{GS}})^{\dagger},
\tag{B.21}
$$

where $(\Phi_{\mathrm{GS}})^{\dagger}$ is calculated the same way as the corresponding expression in hybrid variables. For instance, in above argument, $\Phi_{\mathrm{RNS}} = b = (\frac{1}{\sqrt{32}}e^{-\rho}p^2)_{\mathrm{GS}} = \Phi_{\mathrm{GS}}$, and $\Psi_{\mathrm{RNS}} = (\Phi_{\mathrm{GS}})^{\dagger} = (-\frac{1}{\sqrt{32}}e^{\rho}\bar{p}^2)_{\mathrm{GS}} = -b\gamma^2$, which leads to (B.12).

Some clarifying remarks on the hermitian conjugation rule of RNS variables are in place here. The conformal weights of Φ_{RNS} and Ψ_{RNS} generally differ when evaluated w.r.t. T_{RNS}. The reason for this is the following: as we have reviewed above, in the presence of a background charge, $T^{\dagger} = T - Q\partial j$. If $\mathscr{O}$ is an operator with U(1) charge q, it can be written in the form $\mathscr{O} = \exp(q\int^z j)\mathscr{O}'$ with $\mathscr{O}'$ neutral under j. (Here we have normalized the current according to $j(z)j(w) \sim \frac{1}{(z-w)^2}$.) The hermitian conjugate operator is $\mathscr{O}^{\dagger} = \exp(-q\int^z j)(\mathscr{O}')^{\dagger}$. Its conformal weight measured with $T^{\dagger}$ is the same as that of $\mathscr{O}$ measured with T. One defines the operator $\widetilde{\mathscr{O}} = \exp(q\int^z j)(\mathscr{O}')^{\dagger}$ which has the same U(1) charge and weight (w.r.t. T) as $\mathscr{O}$.

For the case of interest, this means that $T = -\frac{1}{2}(\partial\rho)^2 - \frac{1}{2}(\partial H)^2 + \frac{1}{2}\partial^2\rho + \frac{i}{2}\sqrt{3}\partial^2 H$ becomes $T^{\dagger} = T - \partial^2\rho - i\sqrt{3}\partial^2 H = T - \partial\mathscr{J}$. The conformal weight of Ψ_{RNS} w.r.t. $T^{\dagger}$ is then the same as that of Φ_{RNS} w.r.t. T. It is now straightforward to find that the Ψ_{RNS} corresponding to $\Phi_{GS} = e^{\sigma}$, e^{χ}, and e^{φ}, for example are given (up to overall signs and rescalings) by $e^{\sigma+2\chi-2\varphi}$, $e^{2\sigma+\chi-2\varphi}$, and $e^{2\sigma+2\chi-3\varphi}$, respectively. Finally, we define the operator conjugation $\mathscr{O} \to \widetilde{\mathscr{O}}$ for the case at

hand. We write any operator with ρ-charge p (with respect to the current $\partial\rho$) and $\mathrm{U}(1)_C$-charge q as

$$\mathscr{O} = e^{-p\rho+\frac{iq}{\sqrt{3}}H}\mathscr{O}' = e^{\frac{1}{2}(p+q)\int^z \mathscr{J}} e^{-\frac{1}{2}(3p+q)(\rho+\frac{i}{\sqrt{3}}H)}\mathscr{O}'. \tag{B.22}$$

Then an operator conjugation preserving the conformal w.r.t. to T is defined by

$$\widetilde{\mathscr{O}} = e^{\frac{1}{2}(p+q)\int^z \mathscr{J}} e^{\frac{1}{2}(3p+q)(\rho+\frac{i}{\sqrt{3}}H)}(\mathscr{O}')^\dagger = e^{(2p+q)\rho+(3p+2q)\frac{i}{\sqrt{3}}H}(\mathscr{O}')^\dagger. \tag{B.23}$$

This is the conjugation used in Sect. 2.1.

C Appendix: Vertex Operators

C.1 Massless RNS Vertex Operators

The field redefinition between the RNS and hybrid variables presented in Sect. 2.3 induces a map of the vertex operators of the RNS formulation to those of the hybrid formulation. We first discuss the unintegrated vertex operators for massless states. The field redefinition (18) [or (33) for the right-moving sector of the type IIA string] relates the RNS vertex operators in the large Hilbert space to operators expressed in terms of chiral GS-variables. To obtain the vertex operators in the hybrid variables one needs to perform the additional map (B.2). It can be shown, however, that this map does not affect any of the expressions discussed below. The reason is that at the massless level the unintegrated vertex operators do not depend on p or $\bar{p}$. Furthermore, they contain at least two powers of θ and $\bar{\theta}$ such that the map is trivial as long as the internal part of the vertex operators are primary.

The vertex operators of the bosonic components of the space-time $\mathscr{N} = 2$ multiplets descend from the NSNS and RR sectors of the 10d superstring. The vertex operators in the large Hilbert space are of the general form

$$\mathscr{V}^{(q,\tilde{q})} = |c\xi e^{\alpha\varphi}|^2 \check{\Phi}^{(q,\tilde{q})} W. \tag{C.1}$$

As explained in Sect. 2.4, $\mathscr{V}$ has conformal weight 0 and ghost number 0 with respect to (24). W is the space-time part of the vertex operator; $\Phi^{(q,\tilde{q})}$ are primary fields of $\mathrm{U}(1)_L \times \mathrm{U}(1)_R$ charge $(q, \tilde{q})$ of the internal $c = 9$, $\mathscr{N} = (2, 2)$ SCFT. In what follows, we mainly concentrate on the left-moving part of the vertex operators, which we denote by $\mathscr{V}^{(q)}$. Notice that the charge of $\check{\Phi}^{(q)}$ with respect to $\check{J}_C$ is the same as the one of $\Phi^{(q)}$ defined by (22) with respect to J_C of (21). According to (25), the charge of the vertex operators $\mathscr{V}^{(q)}$ under $J = \partial\rho$ is $-q + 3(1 + \alpha)$ and must therefore carry a factor of $e^{[q-3(1+\alpha)]\rho}$ when expressed in hybrid variables. Since the ghost number $J_{\mathrm{gh}} = \mathscr{J} = \partial\rho + J_C$ of the vertex operator $\mathscr{V}^{(q)}$ is zero, the ρ-charge is minus the J_C-charge. Therefore the internal part of $\mathscr{V}^{(q)}$ in hybrid variables must involve $\Phi^{(q-3[1+\alpha])}$. Given any RNS vertex operator, this rule fixes

the form of the vertex operator in the hybrid formulation up to the spacetime part. The latter is determined by (18) from which one derives, for example,[16]

$$e^{-\rho}\theta^2 = c, \qquad e^{\rho}\bar{\theta}^2 = ce^{-2(\varphi-\chi)}. \tag{C.2}$$

The RNS vertex operators are restricted by the requirement that their operator product with the spacetime gravitino $e^{-\frac{1}{2}\varphi}S^\alpha\Sigma$ is local. This applies to the left-moving part. For the right-moving part of type IIB (IIA) locality with $(e^{-\frac{1}{2}\varphi}S^\alpha\Sigma)_R((e^{-\frac{1}{2}\varphi}S^\alpha\bar{\Sigma})_R)$ is required. Given the OPE $\Sigma(z)\breve{\Phi}^{(q)}(w) \sim (z-w)^{\frac{q}{2}}\breve{\Phi}^{(q+\frac{3}{2})}(w)+\cdots$ this implies restrictions on q.

It is now straightforward to find the following maps of vertex operators in the NS sector in the canonical ghost picture ($\alpha=-1$):[17]

$$\begin{aligned}
\mathscr{V}^{(0)}_{\rm NS} &= c\xi e^{-\varphi}\psi^m(\theta\sigma^m\bar{\theta}),\\
\mathscr{V}^{(+1)}_{\rm NS} &= c\xi e^{-\varphi}\breve{\Phi}^{(+1)} = e^{\rho}\bar{\theta}^2\Phi^{(+1)},\\
\mathscr{V}^{(-1)}_{\rm NS} &= c\xi e^{-\varphi}\breve{\Phi}^{(-1)} = e^{-\rho}\theta^2\Phi^{(-1)}.
\end{aligned} \tag{C.3}$$

In the R sector in the canonical ghost picture ($\alpha=-\frac{1}{2}$) one finds, for example,

$$\begin{aligned}
\mathscr{V}^{(+\frac{3}{2})}_{\rm R} &= c\xi e^{-\frac{\varphi}{2}}S^\alpha\Sigma = \theta^\alpha\bar{\theta}^2,\\
\mathscr{V}^{(+\frac{1}{2})}_{\rm R} &= c\xi e^{-\frac{\varphi}{2}}\bar{S}^{\dot\alpha}\breve{\Phi}^{(+\frac{1}{2})} = e^{-\rho}\bar{\theta}^{\dot\alpha}\theta^2\Phi^{(-1)},\\
\mathscr{V}^{(-\frac{1}{2})}_{\rm R} &= c\xi e^{-\frac{\varphi}{2}}S^\alpha\breve{\Phi}^{(-\frac{1}{2})} = e^{-2\rho}\theta^\alpha\partial\theta^2\Phi^{(-2)}.
\end{aligned} \tag{C.4}$$

These expressions illustrate that RNS vertex operators, which are (RNS) hermitian conjugates of each other, are generally not mapped to operators which are hermitian conjugates in the hybrid sense (cf. Appendix B). Conversely, two hermitian conjugate hybrid operators are related to RNS operators in different ghost pictures. For instance, $\bar{\theta}^{\dot\alpha}\theta^2(w) = c\partial c\xi\partial\xi e^{-\frac{5}{2}\varphi}\bar{S}^{\dot\alpha}\bar{\Sigma}(w) = \lim_{z\to w}Y(z)c\xi e^{-\frac{\varphi}{2}}\bar{S}^{\dot\alpha}\bar{\Sigma}(w)$ where $Y = c\partial\xi e^{-2\varphi}$ is the inverse picture changing operator.

For type IIB compactifications (C.2), (C.3) and (C.4) are the same for both the left- and right-moving sectors. For type IIA compactifications the expressions for the right-movers are different; they can be obtained from above relations by reversing the signs of all explicit charge labels and replacing $\Sigma \leftrightarrow \bar{\Sigma}$.

[16] Here and in what follows we suppress overall signs and numerical factors.

[17] We do not display the $e^{ik\cdot X}$ factors which must be included in the complete expression for each vertex.

C.2 Universal Massless Multiplets

The vertex operators for the universal sector of type II strings on CY_3 [18, 5] are associated to the identity $\Phi^{(0,0)} = \mathbb{1}$ and the states in the RR sector connected to the identity by spectral flow. They are grouped in to the real superfield $\mathscr{U}(x, \theta_{L,R}, \bar{\theta}_{L,R})$, which was constructed in [10], and contains the $24+24$ degrees of freedom of supergravity multiplet and the $8+8$ degrees of freedom of the universal tensor multiplet (which can be dualized to the universal dilaton multiplet). In the Wess-Zumino gauge, the metric, the antisymmetric tensor, and the dilaton appear at the lowest non-vanishing order of the θ-expansion of $\mathscr{U}$. Other fields, such as the (anti)selfdual part of the graviphoton field strength $F_{\alpha\beta}$ ($F_{\dot\alpha\dot\beta}$) and the derivative of the complex RR-scalar Z, to which we referred to in the main text, appear at higher orders in the θ-expansion:

$$\begin{aligned}\mathscr{U} &= \zeta_{mn}(\theta\sigma^m\bar\theta)_L(\theta\sigma^n\bar\theta)_R + \Big[F_{\alpha\beta}\theta_L^\alpha\theta_R^\beta|\bar\theta^2|^2 + \text{h.c.}\Big] \\ &+ \Big[(\partial_{\alpha\dot\beta}Z + \ldots)\theta_L^\alpha\bar\theta_L^2\bar\theta_R^{\dot\beta}\theta_R^2 + \text{h.c.}\Big] + \cdots\end{aligned} \tag{C.5}$$

The full expansion can be found in [10]. Using the expressions (C.3) and (C.4) these operators are identified as the RNS vertex operators. One finds, for instance,

$$\begin{aligned}\mathscr{U}_\zeta &= \zeta_{mn}\psi_L^m\psi_R^n\left|c\xi e^{-\varphi}\right|^2 \\ \mathscr{U}_{\partial Z} &= \partial_m Z(S_L\sigma^m\bar S_R)\left|c\xi e^{-\frac{1}{2}\varphi}\Sigma\right|^2 \\ \mathscr{U}'_{\partial\bar Z} &= \partial_m\bar Z(\bar S_L\sigma^m S_R)\left|c\xi e^{-\frac{1}{2}\varphi}\bar\Sigma\right|^2\end{aligned} \tag{C.6}$$

As explained in the previous section, it is not $\mathscr{U}'_{\partial\bar Z}$ that is mapped directly to the hybrid vertex operator, but the picture changed operator $Y\mathscr{U}'_{\partial\bar Z}$.

C.3 Compactification Dependent Massless Multiplets

The spacetime parts of the massless vertex operators, the presence of which depends on the particular choice of Calabi-Yau compactification, can be grouped into real chiral or twisted-chiral multiplets as described in Sect. 2.5.

Chiral superfields M_c satisfy $\bar D_{\dot\alpha L}M_c = 0 = \bar D_{\dot\alpha R}M_c$. Real chiral superfields (vector multiplets) satisfy in addition $D_L^2M_c = \bar D_R^2\bar M_c$ and comprise $8+8$ components. The chirality constraint means that M_c is a function of $y^m = x^m + i(\theta\sigma^m\bar\theta)_L + i(\theta\sigma^m\bar\theta)_R$, θ_L and θ_R where y^m satisfies $D_Ly^m = \bar D_Ry^m = 0$. Parts of the θ-expansion are

$$M_c(y^m,\theta_L,\theta_R) = t + \cdots + f_{\alpha\beta}\theta_L^\alpha\theta_R^\beta + \cdots + |\theta^2|^2\partial^m\partial_m\bar t', \tag{C.7}$$

where the complex scalars t and t' and the selfdual two-tensor $f_{\alpha\beta}$ are functions of y^m. The reality constraint implies in particular that $t = t'$ and that the two-tensor satisfies the Bianchi constraints, which are solved by writing it as a vector field strength. The complete expansion can be found in [10].

Twisted-chiral superfields M_{tc} satisfy $\bar{D}_{\dot{\alpha}L} M_{tc} = 0 = D_{\alpha R} M_{tc}$. Real twisted-chiral superfields (tensor multiplets) satisfy in addition $D_L^2 M_{tc} = D_R^2 \bar{M}_{tc}$ and comprise $8 + 8$ components. The relevant parts of its expansion are

$$M_{tc}(z, \theta_L, \bar{\theta}_R) = l_{++} + \cdots + v_{\alpha\dot{\beta}} \theta_L^{\alpha} \bar{\theta}_R^{\dot{\beta}} + \cdots + \theta_L^2 \bar{\theta}_R^2 \partial^m \partial_m l_{--}, \tag{C.8}$$

where $v_{\alpha\dot{\beta}} = v_m \sigma^m_{\alpha\dot{\beta}}$ is a complex vector and $l_{\pm\pm}$ complex scalars. All component fields are functions of $z^m = x^m + i(\theta\sigma^m\bar{\theta})_L - i(\theta\sigma^m\bar{\theta})_R$ with $\bar{D}_L z^m = D_R z^m = 0$. The reality condition implies $\bar{l}_{++} = l_{--}$. Its real part requires $\partial_m v_n - \partial_n v_m = 0$ while for its imaginary part we need $\partial^m v_m = 0$. These conditions are solved for $v_m = \partial_m l_{+-} + i\epsilon_{mnpq} H^{npq}$ with $H = dB$. The three scalars $(l_{+-}, l_{--} = \bar{l}_{++})$ form a SU(2) triplet. The antisymmetric tensor with field strength H can be dualized to a fourth scalar which can be combined with l_{+-} to a complex scalar. The complete expansion of this field can again be found in [10].

C.3.1 Kähler Moduli

The $h^{1,1}$ complexified Kähler deformations are in one-to-one correspondence to elements of $H^{1,1}(CY_3)$. In the CFT description they are described by twisted-chiral primaries Ω_{tc} in the (c, a) ring of charge $q_L = -q_R = 1$ and conformal weight $h_L = h_R = \frac{1}{2}$ (in the untwisted theory). They are obtained, via spectral flow, from RR ground states with $q_L = -q_R = -\frac{1}{2}$ and $h_L = h_R = \frac{3}{8}$. In type IIA these deformations are associated with the complex scalars of vector multiplets and for type IIB with the NSNS-scalars of hypermultiplets (or tensor multiplets).

Here, we focus on type IIA, but the generalization to type IIB is straightforward. The corresponding hybrid vertex operators were given in (50)

$$\mathscr{U}_{ca} = |e^{\rho}\bar{\theta}|^2 M_c \Omega_{tc}. \tag{C.9}$$

Note that for the twisted type IIA theory Ω_{tc} has conformal weight $h_L = h_R = 0$ (while $\bar{\Omega}_{tc}$ has conformal weight $h_L = h_R = 1$) such that M_c indeed describes massless states. In the large volume limit the twisted-chiral primary operators can be written as[18]

$$\Omega_{tc} = h_{i\bar{j}} \chi_L^i \chi_R^{\bar{j}}, \qquad \bar{\Omega}_{tc} = h_{i\bar{j}} \lambda_L^{\bar{j}} \lambda_R^i. \tag{C.10}$$

Here $h_{i\bar{j}}$ is an element of $H^{1,1}(CY_3)$. For notational simplicity we drop the additional index which distinguishes between the $h^{1,1}$ different elements.

[18] The left-moving $(\psi_L^i, \psi_L^{\bar{i}})$ are twisted to $(\chi_L^i, \lambda_L^{\bar{i}})$ with conformal weights $(0, 1)$. For the type IIA twist the right-movers $(\psi_R^i, \psi_R^{\bar{i}})$ are twisted to $(\lambda_R^i, \chi_R^{\bar{i}})$ with conformal weight $(1, 0)$.

The bosonic degrees of freedom of the $h^{1,1}$ vector multiplets are found by expanding M_c in powers of θ_L and θ_R,

$$\begin{aligned}\mathscr{U}_t &= t|e^{\rho}\bar{\theta}^2|^2\Omega_{tc},\\ \mathscr{U}_f &= f_{\alpha\beta}\theta_L^{\alpha}\theta_R^{\beta}|e^{\rho}\bar{\theta}^2|^2\Omega_{tc}.\end{aligned}$$

For each Kähler modulus there is a complex polarization t. Its real (imaginary) part is the space-time scalar field corresponding to fluctuations of the internal NSNS B-field $B_{i\bar{j}}$ (mixed components of the CY metric $g_{i\bar{j}}$). $f_{\alpha\beta}$ is the selfdual part of a field strength of the vector multiplet's gauge field which arises from the reduction of the three-form potential. This can be seen by relating these expressions to the vertex operators in the RNS formulation. Using (C.3) and (C.4) one finds

$$\begin{aligned}\mathscr{U}_t &= t|c\xi e^{-\varphi}|^2\breve{\Omega}_{tc},\\ (\mathscr{U}_t)^{\dagger} &= \bar{t}|c\xi e^{-\varphi}|^2\bar{\breve{\Omega}}_{tc},\\ (\mathscr{U}_f)^{\dagger} &= f_{\dot{\alpha}\dot{\beta}}\bar{S}_L^{\dot{\alpha}}\bar{S}_R^{\dot{\beta}}|c\xi e^{-\frac{1}{2}\varphi}|^2\bar{\breve{\Omega}}_{tc}.\end{aligned} \tag{C.11}$$

Incidentally, the choice in (18) is such that $(\mathscr{U}_f)^{\dagger}$ is mapped to a simple RNS vertex operator in the canonical ghost picture while $\mathscr{U}_f$ is mapped to a RNS operator in another ghost picture.

C.3.2 Complex Structure Moduli

The $h^{2,1}$ complex structure deformations are related to chiral primary fields Ω_c in the chiral (c,c) ring of charge $q_L = q_R = 1$ and conformal weight $h_L = h_R = \frac{1}{2}$ (in the untwisted theory). These are related to operators describing RR ground states with charges $q_L = q_R = \pm\frac{1}{2}$ and $h_L = h_R = \frac{3}{8}$ by spectral flow. Again, we focus on the type IIA string, in which case they correspond to the NSNS scalars in hypermultiplets, other than the universal one which contains the dilaton. In the hybrid formalism the space-time part of these states is described by a real twisted-chiral multiplet M_{tc} with the field content of a tensor multiplet. The vertex operators are contained in the potentials given in (50)

$$\mathscr{U}_{cc} = e^{\rho_L-\rho_R}\bar{\theta}_L^2\theta_R^2 M_{tc}\Omega_c. \tag{C.12}$$

The chiral primary field Ω_c has conformal weight $h_L = 0$ and $h_R = 1$ (while $\bar{\Omega}_c$ has weights $h_L = 1$ and $h_R = 0$) such that M_{tc} indeed describes massless states. In the large volume limit one has

$$\Omega_c = h_{ij}\chi_L^i\lambda_R^j, \qquad \bar{\Omega}_c = h_{\bar{\imath}\bar{\jmath}}\lambda_L^{\bar{\imath}}\chi_R^{\bar{\jmath}}, \tag{C.13}$$

where $h_{ij} = g_{j\bar{j}} h_i{}^{\bar{j}}$, and $h_i{}^{\bar{j}}$ is related to elements $Y_{i\bar{j}\bar{k}} h_i{}^{\bar{i}} \bar{\Omega}_{\bar{i}\bar{j}\bar{k}}$ of $H^{1,2}(CY_3)$. Again, we suppress the index that distinguishes between these $h^{2,1}$ different elements.

The vertex operators contained in this multiplet can be extracted by expanding M_{tc} in powers of θ_L and $\bar{\theta}_R$. The lowest components are

$$\begin{aligned} \mathscr{U}_{l_{++}} &= l_{++} e^{\rho_L - \rho_R} \bar{\theta}_L^2 \theta_R^2 \Omega_c, \\ \mathscr{U}_v &= v_{\alpha\dot{\beta}} \theta_L^{\alpha} \bar{\theta}_R^{\dot{\beta}} e^{\rho_L - \rho_R} \bar{\theta}_L^2 \theta_R^2 \Omega_c. \end{aligned} \tag{C.14}$$

The scalar l_{++} parameterizes the fluctuations $h_{ij} = g_{j\bar{j}} h_i^{\bar{j}}$ of the pure components of the internal graviton g_{ij}. The complex polarization v_m is related to the internal components of the RR 3-form as $C_{ij\bar{k}} CY_{ij\bar{k}}$. The complex scalar C can be expressed by the real scalar l_{+-} and the dual of a real two-form field strength H_{mnp} such that $v_m = \partial_m C = (\partial_m l_{+-} + i\epsilon_{mnpq} H^{npq})$. Reducing the RNS vertex operators for the type IIA RR three-form and of the internal graviton one finds, in agreement with (C.3) and (C.4),

$$\begin{aligned} \mathscr{U}_{l_{++}} &= l_{++} |c\xi e^{-\varphi}|^2 \breve{\Omega}_c, \\ (\mathscr{U}_v)^{\dagger} &= \bar{v}_{\dot{\alpha}\beta} \bar{S}_L^{\dot{\alpha}} S_R^{\beta} |c\xi e^{-\frac{\varphi}{2}}|^2 \bar{\breve{\Omega}}_c. \end{aligned} \tag{C.15}$$

As for the Kähler moduli, the operator $\mathscr{U}_v$ maps to a RNS vertex operator in a non-canonical ghost-picture.

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Quantum Phases of Cold Bosons in an Optical Lattice*

Michael Aizenman, Elliot H. Lieb, Robert Seiringer, Jan Philip Solovej and Jakob Yngvason

Abstract In recent years it has become possible to trap ultracold atoms and molecules in lattices generated by laser beams (optical lattices). By varying the experimentally tunable parameters transitions between various phases of the trapped gas, in particular between a Bose-Einstein condensate and a Mott insulator phase, can be produced. Theoretical investigations of this phenomenon are mostly based on variational or numerical studies of a Bose-Hubbard model but a rigorous proof of a phase transition in this model is still lacking. There exists, however, a related model where such a phenomenon can be analysed rigorously. This is the hard core lattice gas where the optical lattice is modeled by a periodic potential of strength λ. For small λ and temperature Bose-Einstein condensation (BEC) is proved to occur, while at large λ BEC disappears, even in the ground state, which is a Mott insulator state

Michael Aizenman
Departments of Mathematics and Physics, Jadwin Hall, Princeton University, P.O. Box 708, Princeton, NJ 08544, USA, e-mail: aizenman@princeton.edu

Elliot H. Lieb
Departments of Mathematics and Physics, Jadwin Hall, Princeton University, P.O. Box 708, Princeton, NJ 08544, USA, e-mail: lieb@princeton.edu

Robert Seiringer
Departments of Mathematics and Physics, Jadwin Hall, Princeton University, P.O. Box 708, Princeton, NJ 08544, USA, e-mail: rseiring@princeton.edu

Jan Philip Solovej
Department of Mathematics, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen, Denmark, e-mail: solovej@math.ku.dk

Jakob Yngvason
Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Vienna, Austria and
Erwin Schrödinger Institute for Mathematical Physics, Boltzmanngasse 9, 1090 Vienna, Austria, e-mail: jakob.yngvason@univie.ac.at

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with a characteristic gap. The inter-particle interaction is essential for this effect. This contribution gives a pedagogical survey of these results.

1 Introduction

Recent experiments [18, 19] with ultra-cold quantum gases in optical traps have verified a prediction [12, 21] of a reversible transition between a Bose-Einstein condensate and a state composed of localized atoms as the strength of a periodic trapping potential is varied. This is an example of a quantum phase transition [32] where quantum fluctuations and correlations rather than energy-entropy competition is the driving force and its theoretical understanding is quite challenging. The model usually considered for describing this phenomenon is the Bose-Hubbard model and a transition between a superfluid and a *Mott insulator* in this model was originally suggested in [12] with an application to He^4 in porous media in mind. The possibility of applying this scheme to a gas of alkali atoms in a periodic potential generated by laser beams ('optical lattice') was first realized in [21]. The articles [37, 4, 20, 26, 5] review these and some of the subsequent developments. The physics of cold atoms in optical lattices has now become a major research subject and it is impossible to do justice here to the large number of papers devoted to this topic that have appeared. As a representative sample we mention only [35, 36, 8, 17, 28, 6, 3, 33, 7, 27, 31, 34, 24] where further references can be found.

Physically, we are dealing with a trapped Bose gas with short range interaction. The model used in the cited papers, however, is not a continuum model but rather a lattice gas, i.e., the particles are confined to move on a d-dimensional, hyper-cubic lattice and the kinetic energy is given by the discrete Laplacian. In terms of bosonic creation and annihilation operators, $a_{\mathbf{x}}^\dagger$ and $a_{\mathbf{x}}$, the Hamiltonian of the Bose-Hubbard model is

$$H_{\mathrm{BH}} = -\frac{1}{2}\sum_{\langle \mathbf{xy}\rangle}\left(a_{\mathbf{x}}^\dagger a_{\mathbf{y}} + a_{\mathbf{x}} a_{\mathbf{y}}^\dagger\right) + U\sum_{\mathbf{x}} a_{\mathbf{x}}^\dagger a_{\mathbf{x}}\left(a_{\mathbf{x}}^\dagger a_{\mathbf{x}} - 1\right). \tag{1}$$

The sites $\mathbf{x}$ are in a cube $\Lambda \subset \mathbb{Z}^d$ with opposite sides identified (i.e., a d-dimensional torus) and $\langle \mathbf{xy}\rangle$ stands for pairs of nearest neighbors. The first term in (2) is the discrete Laplacian $\sum_{\langle \mathbf{xy}\rangle}(a_{\mathbf{x}}^\dagger - a_{\mathbf{y}}^\dagger)(a_{\mathbf{x}} - a_{\mathbf{y}})$ minus $2d\sum_{\mathbf{x}} a_{\mathbf{x}}^\dagger a_{\mathbf{x}}$, i.e., we have subtracted a chemical potential that equals d. Units are chosen such that the hopping parameter in front of the kinetic term is $1/2$.

The investigations of a phase transition in the Bose-Hubbard model as the interatomic on-site repulsion U is varied are mostly based on variational or numerical methods. The signal of the phase transition is usually taken to be that an ansatz with a sharp particle number at each lattice site leads to a lower energy than a delocalized Bogoliubov state. There are several papers, e.g., [13, 10] and the recent paper [11], where rigorous results are obtained by other methods, but so far there exists no proof that the true ground state of the model has off-diagonal long range order at one end

of the parameter regime that disappears at the other end. In the present contribution, which is based on the paper [2], we study a slightly different model where just this phenomenon can be rigorously proved and which, at the same time, captures the salient features of the experimental situation.

Our model is that of a *hard-core lattice gas* which corresponds formally to $U = \infty$ in the Bose-Hubbard model. The optical lattice is modeled by a periodic, one-body potential, whose strength is measured by an adjustable parameter λ. Instead of (1) we thus consider the Hamiltonian

$$H = -\frac{1}{2}\sum_{\langle \mathbf{xy}\rangle}\left(a_{\mathbf{x}}^{\dagger}a_{\mathbf{y}} + a_{\mathbf{x}}a_{\mathbf{y}}^{\dagger}\right) + \lambda\sum_{\mathbf{x}}(-1)^{\mathbf{x}}a_{\mathbf{x}}^{\dagger}a_{\mathbf{x}}. \tag{2}$$

The operators $a_{\mathbf{x}}^{\#}$ in this model commute at different sites as appropriate for Bosons but satisfy anti-commutation relations on the same site, reflecting the hard-core condition. When discussing BEC, it is convenient not to fix the particle number but to work in a grand-canonical ensemble. The chemical potential is fixed in such a way that the average particle number equals half the number of lattice sites, i.e., we consider *half filling*. (This restriction is dictated by our method of proof.) In experiments the gas is enclosed in an additional trap potential that is slowly varying on the scale of the optical lattice but we neglect here the inhomogeneity due to such a potential and consider instead the thermodynamic limit.

The optical lattice gives rise to the potential $\lambda(-1)^{\mathbf{x}}$ which alternates in sign between the A and B sublattices of even and odd sites. In the Bose-Hubbard model, on the other hand, all sites are equivalent and the lattice represents only the attractive sites of the optical lattice. In our case the adjustable parameter is λ instead of U and for large λ the atoms will try to localize on the B sublattice. Because of the periodic potential the unit cell in our model consists of two lattice sites, so that we have on average one particle per unit cell. This corresponds, physically, to filling factor 1 in the Bose-Hubbard model.

The Hamiltonian (2) conserves the particle number N and it is shown in [2], Appendix A, that the lowest energy is obtained uniquely for $N = \frac{1}{2}|\Lambda|$, i.e., half the number of lattice sites.

For given temperature T, we consider grand-canonical thermal equilibrium states, described by the Gibbs density matrices $Z^{-1}\exp(-\beta H)$ with Z the normalization factor (partition function) and $\beta = 1/T$ the inverse temperature. Units are chosen so that Boltzmann's constant equals 1. The thermal expectation value of some observable $\mathscr{O}$ will be denoted by $\langle\mathscr{O}\rangle = Z^{-1}\,\mathrm{Tr}\,\mathscr{O}\exp(-\beta H)$. In the proof of BEC we focus on dimensions $d \geq 3$, but, using the technique employed in [22], an extension to the ground state in two dimensions is possible.

Our main results about this model can be summarized as follows:

1. If T and λ are both small, there is Bose-Einstein condensation. In this parameter regime the one-body density matrix $\gamma(\mathbf{x},\mathbf{y}) = \langle a_{\mathbf{x}}^{\dagger}a_{\mathbf{y}}\rangle$ has exactly one large eigenvalue (in the thermodynamic limit), and the corresponding condensate wave function is $\phi(\mathbf{x}) =$ constant.

2. If either T or λ is big enough, then the one-body density matrix decays exponentially with the distance $|\mathbf{x}-\mathbf{y}|$, and hence there is *no BEC*. In particular, this applies to the ground state $T=0$ for λ big enough, where the system is in a Mott insulator phase.
3. The Mott insulator phase is characterized by a gap, i.e., a jump in the chemical potential. We are able to prove this, at half-filling, in the region described in item 2 above. More precisely, there is a cusp in the dependence of the ground state energy on the number of particles; adding or removing one particle costs a non-zero amount of energy. We also show that there is no such gap whenever there is BEC.
4. The interparticle interaction is essential for items 2 and 3. Non-interacting bosons *always display BEC* for sufficiently low, but positive T (depending on λ, of course).
5. For all $T \geq 0$ and all $\lambda > 0$ the diagonal part of the one-body density matrix $\langle a_{\mathbf{x}}^{\dagger} a_{\mathbf{x}} \rangle$ (the one-particle density) is *not constant*. Its value on the A sublattice is constant, but strictly less than its constant value on the B sublattice and this discrepancy survives in the thermodynamic limit. In contrast, in the regime mentioned in item 1, the off-diagonal long-range order is constant, i.e., $\langle a_{\mathbf{x}}^{\dagger} a_{\mathbf{y}} \rangle \approx \phi(\mathbf{x})\phi(\mathbf{y})^*$ for large $|\mathbf{x}-\mathbf{y}|$ with $\phi(\mathbf{x}) =$ constant.

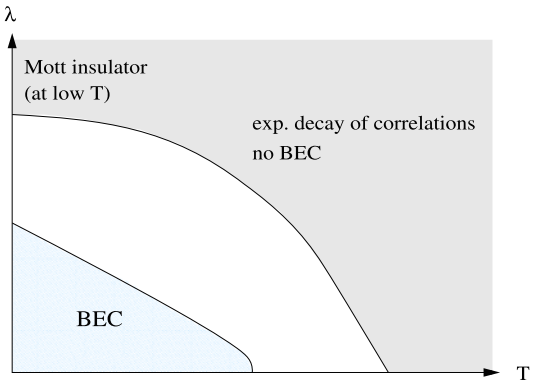

Fig. 1 Schematic phase diagram at half-filling

Because of the hard-core interaction between the particles, there is at most one particle at each site and our Hamiltonian (2) thus acts on the Hilbert space $\mathscr{H} = \bigotimes_{\mathbf{x}\in\Lambda} \mathbb{C}^2$. The creation and annihilation operators can be represented as 2×2 matrices with

$$a_{\mathbf{x}}^{\dagger} \leftrightarrow \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad a_{\mathbf{x}} \leftrightarrow \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \qquad a_{\mathbf{x}}^{\dagger} a_{\mathbf{x}} \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},$$

for each $\mathbf{x} \in \Lambda$. More precisely, these matrices act on the tensor factor associated with the site $\mathbf{x}$ while $a_{\mathbf{x}}^\dagger$ and $a_{\mathbf{x}}$ act as the identity on the other factors in the Hilbert space $\mathscr{H} = \bigotimes_{\mathbf{x}\in\Lambda} \mathbb{C}^2$.

The Hamiltonian can alternatively be written in terms of the spin 1/2 operators

$$S^1 = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad S^2 = \frac{1}{2}\begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \qquad S^3 = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The correspondence with the creation and annihilation operators is

$$a_{\mathbf{x}}^\dagger = S_{\mathbf{x}}^1 + \mathrm{i}S_{\mathbf{x}}^2 \equiv S_{\mathbf{x}}^+, \qquad a_{\mathbf{x}} = S_{\mathbf{x}}^1 - \mathrm{i}S_{\mathbf{x}}^2 \equiv S_{\mathbf{x}}^-,$$

and hence $a_{\mathbf{x}}^\dagger a_{\mathbf{x}} = S_{\mathbf{x}}^3 + \frac{1}{2}$. (This is known as the Matsubara-Matsuda correspondence [25].) Adding a convenient constant to make the periodic potential positive, the Hamiltonian (2) is thus equivalent to

$$\begin{aligned} H &= -\frac{1}{2}\sum_{\langle \mathbf{xy}\rangle}\left(S_{\mathbf{x}}^+ S_{\mathbf{y}}^- + S_{\mathbf{x}}^- S_{\mathbf{y}}^+\right) + \lambda \sum_{\mathbf{x}}\left[\frac{1}{2} + (-1)^{\mathbf{x}} S_{\mathbf{x}}^3\right] \\ &= -\sum_{\langle \mathbf{xy}\rangle}\left(S_{\mathbf{x}}^1 S_{\mathbf{y}}^1 + S_{\mathbf{x}}^2 S_{\mathbf{y}}^2\right) + \lambda \sum_{\mathbf{x}}\left[\frac{1}{2} + (-1)^{\mathbf{x}} S_{\mathbf{x}}^3\right]. \end{aligned} \tag{3}$$

Without loss of generality we may assume $\lambda \geq 0$. This Hamiltonian is well known as a model for interacting spins, referred to as the XY model [9]. The last term has the interpretation of a staggered magnetic field. We note that BEC for the lattice gas is equivalent to off-diagonal long range order for the 1- and 2-components of the spins.

The Hamiltonian (3) is clearly invariant under simultaneous rotations of all the spins around the 3-axis. In particle language this is the $U(1)$ gauge symmetry associated with particle number conservation of the Hamiltonian (2). Off-diagonal long range order (or, equivalently, BEC) implies that this symmetry is spontaneously broken in the state under consideration, cf., e.g. [23]. It is notoriously difficult to prove such symmetry breaking for systems with a continuous symmetry. One of the few available techniques is that of *reflection positivity* (and the closely related property of *Gaussian domination*) and fortunately it can be applied to our system. For this, however, the hard core and half-filling conditions are essential because they imply a particle-hole symmetry that is crucial for the proofs to work. Naturally, BEC is expected to occur at other fillings, but no one has so far found a way to prove condensation (or, equivalently, long-range order in an antiferromagnet with continuous symmetry) without using reflection positivity and infrared bounds, and these require the additional symmetry.

Reflection positivity was first formulated by K. Osterwalder and R. Schrader [29, 30] in the context of relativistic quantum field theory. Later, J. Fröhlich, B. Simon and T. Spencer used the concept to prove the existence of a phase transition for a classical spin model with a continuous symmetry [16, 15], and E. Lieb and J. Fröhlich [14] as well as F.J. Dyson, E.H. Lieb and B. Simon [9] applied it for the analysis of quantum spin systems. The proof of off-diagonal long range order for

the Hamiltonian (3) (for small λ) given here is based on appropriate modifications of the arguments in [9].

2 Reflection Positivity

In the present context reflection positivity means the following. We divide the torus Λ into two congruent parts, Λ_{L} and Λ_{R}, by cutting it with a hyperplane orthogonal to one of the d directions. (For this we assume that the side length of Λ is even.) This induces a factorization of the Hilbert space, $\mathscr{H} = \mathscr{H}_{\mathrm{L}} \otimes \mathscr{H}_{\mathrm{R}}$, with

$$\mathscr{H}_{\mathrm{L,R}} = \bigotimes_{\mathbf{x}\in\Lambda_{\mathrm{L,R}}} \mathbb{C}^2.$$

There is a natural identification between a site $\mathbf{x} \in \Lambda_{\mathrm{L}}$ and its mirror image $\vartheta\mathbf{x} \in \Lambda_{\mathrm{R}}$. If F is an operator on $\mathscr{H} = \mathscr{H}_{\mathrm{L}}$ we define its reflection θF as an operator on $\mathscr{H}_{\mathrm{R}}$ in the following way. If $F = F_{\mathbf{x}}$ operates non-trivially only on one site, $\mathbf{x} \in \Lambda_{\mathrm{L}}$, we define $\theta F = V F_{\vartheta\mathbf{x}} V^\dagger$ where V denotes the unitary particle-hole transformation or, in the spin language, rotation by π around the 1-axis. This definition extends in an obvious way to products of operators on single sites and then, by linearity, to arbitrary operators on $\mathscr{H}_{\mathrm{L}}$. Reflection positivity of a state $\langle\cdot\rangle$ means that

$$\langle F\theta\overline{F}\rangle \geq 0 \tag{4}$$

for any F operating on $\mathscr{H}_{\mathrm{L}}$. Here $\overline{F}$ is the complex conjugate of the operator F in the matrix representation defined above, i.e., defined by the basis where the operators $S^3_{\mathbf{x}}$ are diagonal.

We now show that reflection positivity holds for any thermal equilibrium state of our Hamiltonian. We can write the Hamiltonian (3) as

$$H = H_{\mathrm{L}} + H_{\mathrm{R}} - \frac{1}{2}\sum_{\langle\mathbf{xy}\rangle\in M}\left(S^+_{\mathbf{x}}S^-_{\mathbf{y}} + S^-_{\mathbf{x}}S^+_{\mathbf{y}}\right), \tag{5}$$

where H_{L} and H_{R} act non-trivially only on $\mathscr{H}_{\mathrm{L}}$ and $\mathscr{H}_{\mathrm{R}}$, respectively. Here, M denotes the set of bonds going from the left sublattice to the right sublattice. (Because of the periodic boundary condition these include the bonds that connect the right boundary with the left boundary.) Note that $H_{\mathrm{R}} = \theta H_{\mathrm{L}}$, and

$$\sum_{\langle\mathbf{xy}\rangle\in M}\left(S^+_{\mathbf{x}}S^-_{\mathbf{y}} + S^-_{\mathbf{x}}S^+_{\mathbf{y}}\right) = \sum_{\langle\mathbf{xy}\rangle\in M}\left(S^+_{\mathbf{x}}\theta S^+_{\mathbf{x}} + S^-_{\mathbf{x}}\theta S^-_{\mathbf{x}}\right).$$

For these properties it is essential that we included the unitary particle-hole transformation V in the definition of the reflection θ. For reflection positivity it is also important that all operators appearing in H (5) have a *real* matrix representation. Moreover, the minus sign in (5) is essential.

Using the Trotter product formula, we have

$$\operatorname{Tr} F\theta\overline{F}e^{-\beta H} = \lim_{n\to\infty} \operatorname{Tr} F\theta\overline{F}\mathscr{Z}_n$$

with

$$\mathscr{Z}_n = \left[e^{-\frac{1}{n}\beta H_L}\theta e^{-\frac{1}{n}\beta H_L} \prod_{\langle \mathbf{xy}\rangle \in M} \left(1 + \frac{\beta}{2n}\left[S^+_{\mathbf{x}}\theta S^+_{\mathbf{x}} + S^-_{\mathbf{x}}\theta S^-_{\mathbf{x}}\right]\right)\right]^n . \tag{6}$$

Observe that $\mathscr{Z}_n$ is a sum of terms of the form

$$\prod_i A_i\theta A_i , \tag{7}$$

with A_i given by either $e^{-\frac{1}{n}\beta H_L}$ or $\sqrt{\frac{\beta}{2n}}S^+_{\mathbf{x}}$ or $\sqrt{\frac{\beta}{2n}}S^-_{\mathbf{x}}$. All the A_i are real matrices, and therefore

$$\operatorname{Tr}_{\mathscr{H}} F\theta\overline{F}\prod_i A_i\theta A_i = \operatorname{Tr}_{\mathscr{H}} F\prod_i A_i\theta\left[\overline{F}\prod_j A_j\right] = \left|\operatorname{Tr}_{\mathscr{H}_{\mathrm{L}}} F\prod_i A_i\right|^2 \geq 0. \tag{8}$$

Hence $\operatorname{Tr} F\theta\overline{F}\mathscr{Z}_n$ is a sum of non-negative terms and therefore non-negative. This proves our assertion.

3 Proof of BEC for Small λ and T

The main tool in our proof of BEC are *infrared bounds*. More precisely, for $\mathbf{p} \in \Lambda^*$ (the dual lattice of Λ), let $\widetilde{S}^{\#}_{\mathbf{p}} = |\Lambda|^{-1/2}\sum_{\mathbf{x}} S^{\#}_{\mathbf{x}}\exp(\mathrm{i}\mathbf{p}\cdot\mathbf{x})$ denote the Fourier transform of the spin operators. We claim that

$$\left(\widetilde{S}^1_{\mathbf{p}}, \widetilde{S}^1_{-\mathbf{p}}\right) \leq \frac{T}{2E_{\mathbf{p}}}, \tag{9}$$

with $E_{\mathbf{p}} = \sum_{i=1}^d (1-\cos(p_i))$. Here, p_i denotes the components of $\mathbf{p}$, and $(\,,\,)$ denotes the Duhamel two point function at temperature T, defined by

$$(A, B) = \int_0^1 \operatorname{Tr}\left(Ae^{-s\beta H}Be^{-(1-s)\beta H}\right) ds / \operatorname{Tr} e^{-\beta H} \tag{10}$$

for any pair of operators A and B. Because of invariance under rotations around the S^3 axis, (9) is equally true with S^1 replaced by S^2, of course.

The crucial lemma (*Gaussian domination*) is the following. Define, for a complex valued function h on the bonds $\langle \mathbf{xy}\rangle$ in Λ,

$$Z(h) = \mathrm{Tr}\exp\left[-\beta K(h)\right], \tag{11}$$

with $K(h)$ the modified Hamiltonian

$$K(h) = \frac{1}{4}\sum_{\langle \mathbf{xy}\rangle}\left(\left(S^+_{\mathbf{x}} - S^-_{\mathbf{y}} - h_{\mathbf{xy}}\right)^2 + \left(S^-_{\mathbf{x}} - S^+_{\mathbf{y}} - \overline{h_{\mathbf{xy}}}\right)^2\right) + \lambda\sum_{\mathbf{x}}\left[\frac{1}{2} + (-1)^{\mathbf{x}}S^3_{\mathbf{x}}\right]. \tag{12}$$

Note that for $h \equiv 0$, $K(h)$ agrees with the Hamiltonian H, because $(S^{\pm})^2 = 0$. We claim that, for any *real valued* h,

$$Z(h) \le Z(0). \tag{13}$$

The infrared bound then follows from $d^2Z(\varepsilon h)/d\varepsilon^2|_{\varepsilon=0} \le 0$, taking $h_{\mathbf{xy}} = \exp(\mathrm{i}\mathbf{p}\cdot\mathbf{x}) - \exp(\mathrm{i}\mathbf{p}\cdot\mathbf{y})$. This is not a real function, though, but the negativity of the (real!) quadratic form $d^2Z(\varepsilon h)/d\varepsilon^2|_{\varepsilon=0}$ for real h implies negativity also for complex-valued h.

The proof of (13) is very similar to the proof of the reflection positivity property (4) given above. It follows along the same lines as in [9], but we repeat it here for convenience of the reader.

The intuition behind (13) is the following. First, in maximizing $Z(h)$ one can restrict to gradients, i.e., $h_{\mathbf{xy}} = \hat{h}_{\mathbf{x}} - \hat{h}_{\mathbf{y}}$ for some function $\hat{h}_{\mathbf{x}}$ on Λ. (This follows from stationarity of $Z(h)$ at a maximizer $h_{\max}$.) Reflection positivity implies that $\langle A\theta\overline{B}\rangle$ defines a scalar product on operators on $\mathscr{H}_{\mathrm{L}}$, and hence there is a corresponding Schwarz inequality. Moreover, since reflection positivity holds for reflections across *any* hyperplane, one arrives at the so-called *chessboard inequality*, which is simply a version of Schwarz's inequality for multiple reflections across different hyperplanes. Such a chessboard estimate implies that in order to maximize $Z(h)$ it is best to choose the function $\hat{h}_{\mathbf{x}}$ to be constant. In the case of classical spin systems [16, 15], this intuition can be turned into a complete proof of (13). Because of non-commutativity of $K(h)$ with $K(0) = H$, this is not possible in the quantum case. However, one can proceed by using the Trotter formula as follows.

Let $h_{\max}$ be a function that maximizes $Z(h)$ for real valued h. If there is more than one maximizer, we choose $h_{\max}$ to be one that vanishes on the largest number of bonds. We then have to show that actually $h_{\max} \equiv 0$. If $h_{\max} \not\equiv 0$, we draw a hyperplane such that $h_{\mathbf{xy}} \neq 0$ for at least one pair $\langle\mathbf{xy}\rangle$ crossing the plane. We can again write

$$K(h) = K_L(h) + K_R(h) + \frac{1}{4}\sum_{\langle\mathbf{xy}\rangle\in M}\left(\left(S^+_{\mathbf{x}} - S^-_{\mathbf{y}} - h_{\mathbf{xy}}\right)^2 + \left(S^-_{\mathbf{x}} - S^+_{\mathbf{y}} - h_{\mathbf{xy}}\right)^2\right). \tag{14}$$

Using the Trotter formula, we have $Z(h) = \lim_{n\to\infty}\alpha_n$, with

$$\alpha_n = \mathrm{Tr}\left[e^{-\beta K_L/n} e^{-\beta K_R/n} \prod_{\langle \mathbf{xy}\rangle \in M} e^{-\beta (S^+_{\mathbf{x}} - S^-_{\mathbf{y}} - h_{\mathbf{xy}})^2/4n} e^{-\beta (S^-_{\mathbf{x}} - S^+_{\mathbf{y}} - h_{\mathbf{xy}})^2/4n} \right]^n . \tag{15}$$

For any matrix, we can write

$$e^{-D^2} = (4\pi)^{-1/2} \int_{\mathbb{R}} dk\, e^{\mathrm{i}kD} e^{-k^2/4}. \tag{16}$$

We apply this to the last two factors in (15), noting that $S^-_{\mathbf{y}} = \theta S^+_{\mathbf{x}}$ if $\langle \mathbf{xy}\rangle \in M$. Denoting by $\mathbf{x}_1, \ldots, \mathbf{x}_l$ the points on the left side of the bonds in M, we then have

$$\begin{aligned} \alpha_n = (4\pi)^{-nl} \int_{R^{2nl}} d^{2nl}k\, \mathrm{Tr}\left[e^{-\beta K_L/n} e^{-\beta K_R/n} e^{\mathrm{i}k_1 (S^+_{\mathbf{x}_1} - \theta S^+_{\mathbf{x}_1})\beta^{1/2}/2n^{1/2}} \ldots \right] \\ \times e^{-k^2/4} e^{-\mathrm{i}k_1 h_{\mathbf{x}_1 \vartheta \mathbf{x}_1} \beta^{1/2}/2n^{1/2}} \ldots . \end{aligned} \tag{17}$$

Here we denote $k^2 = \sum k_i^2$ for short. Since matrices on the right of M commute with matrices on the left, and since all matrices in question are *real*, we see that the trace in the integrand above can be written as

$$\mathrm{Tr}\left[e^{-\beta K_L/n} e^{\mathrm{i}k_1 S^+_{\mathbf{x}_1}\beta^{1/2}/2n^{1/2}} \ldots \right] \overline{\mathrm{Tr}\left[e^{-\beta K_R/n} e^{\mathrm{i}k_1 \theta S^+_{\mathbf{x}_1}\beta^{1/2}/2n^{1/2}} \ldots \right]}. \tag{18}$$

Using the Schwarz inequality for the k integration, and 'undoing' the above step, we see that

$$\begin{aligned} |\alpha_n|^2 \le \Bigg((4\pi)^{-nl} \int_{R^{2nl}} d^{2nl}k\, e^{-k^2/4} \\ \times \mathrm{Tr}\left[e^{-\beta K_L/n} e^{-\beta\theta K_L/n} e^{\mathrm{i}k_1 (S^+_{\mathbf{x}_1} - \theta S^+_{\mathbf{x}_1})\beta^{1/2}/2n^{1/2}} \ldots \right] \Bigg) \\ \times \Bigg((4\pi)^{-nl} \int_{R^{2nl}} d^{2nl}k\, e^{-k^2/4} \\ \times \mathrm{Tr}\left[e^{-\beta\theta K_R/n} e^{-\beta K_R/n} e^{\mathrm{i}k_1 (S^+_{\mathbf{x}_1} - \theta S^+_{\mathbf{x}_1})\beta^{1/2}/2n^{1/2}} \ldots \right] \Bigg). \end{aligned} \tag{19}$$

In terms of the partition function $Z(h)$, this means that

$$|Z(h_{\max})|^2 \le Z(h^{(1)}) Z(h^{(2)}), \tag{20}$$

where $h^{(1)}$ and $h^{(2)}$ are obtained from $h_{\max}$ by reflection across M in the following way:

$$h^{(1)}_{\mathbf{xy}} = \begin{cases} h_{\mathbf{xy}} & \text{if } \mathbf{x}, \mathbf{y} \in \Lambda_{\mathrm{L}} \\ h_{\vartheta \mathbf{x} \vartheta \mathbf{y}} & \text{if } \mathbf{x}, \mathbf{y} \in \Lambda_{\mathrm{R}} \\ 0 & \text{if } \langle \mathbf{xy}\rangle \in M \end{cases} \tag{21}$$

and $h^{(2)}$ is given by the same expression, interchanging L and R. Therefore also $h^{(1)}$ and $h^{(2)}$ must be maximizers of $Z(h)$. However, one of them will contain strictly more zeros than $h_{\max}$, since $h_{\max}$ does not vanish identically for bonds crossing M. This contradicts our assumption that $h_{\max}$ contains the maximal number of zeros among all maximizers of $Z(h)$. Hence $h_{\max} \equiv 0$ identically. This completes the proof of (13).

The next step is to transfer the upper bound on the Duhamel two point function (9) into an upper bound on the thermal expectation value. This involves convexity arguments and estimations of double commutators like in Sect. 3 in [9]. For this purpose, we have to evaluate the double commutators

$$\big[\widetilde{S}^1_{\mathbf{p}}, \big[H, \widetilde{S}^1_{-\mathbf{p}}\big]\big] + \big[\widetilde{S}^2_{\mathbf{p}}, [H, \widetilde{S}^2_{-\mathbf{p}}]\big] = -\frac{2}{|\Lambda|}\bigg(H - \frac{1}{2}\lambda|\Lambda| + 2\sum_{\langle \mathbf{xy}\rangle} S^3_{\mathbf{x}} S^3_{\mathbf{y}} \cos \mathbf{p}\cdot(\mathbf{x}-\mathbf{y})\bigg). \tag{22}$$

Let $C_{\mathbf{p}}$ denote the expectation value of this last expression,

$$C_{\mathbf{p}} = \big\langle \big[\widetilde{S}^1_{\mathbf{p}}, \big[H, \widetilde{S}^1_{-\mathbf{p}}\big]\big] + \big[\widetilde{S}^2_{\mathbf{p}}, \big[H, \widetilde{S}^2_{-\mathbf{p}}\big]\big]\big\rangle \geq 0.$$

The positivity of $C_{\mathbf{p}}$ can be seen from an eigenfunction-expansion of the trace. From [9, Corollary 3.2 and Theorem 3.2] and (9) we infer that

$$\big\langle \widetilde{S}^1_{\mathbf{p}} \widetilde{S}^1_{-\mathbf{p}} + \widetilde{S}^2_{\mathbf{p}} \widetilde{S}^2_{-\mathbf{p}} \big\rangle \leq \frac{1}{2}\sqrt{\frac{C_{\mathbf{p}}}{E_{\mathbf{p}}}} \coth \sqrt{\beta^2 C_{\mathbf{p}} E_{\mathbf{p}}/4}. \tag{23}$$

Using $\coth x \leq 1 + 1/x$ and Schwarz's inequality, we obtain for the sum over all $\mathbf{p} \neq \mathbf{0}$,

$$\sum_{\mathbf{p}\neq\mathbf{0}} \big\langle \widetilde{S}^1_{\mathbf{p}} \widetilde{S}^1_{-\mathbf{p}} + \widetilde{S}^2_{\mathbf{p}} \widetilde{S}^2_{-\mathbf{p}} \big\rangle \leq \frac{1}{\beta}\sum_{\mathbf{p}\neq\mathbf{0}} \frac{1}{E_{\mathbf{p}}} + \frac{1}{2}\bigg(\sum_{\mathbf{p}\neq\mathbf{0}} \frac{1}{E_{\mathbf{p}}}\bigg)^{1/2} \bigg(\sum_{\mathbf{p}\neq\mathbf{0}} C_{\mathbf{p}}\bigg)^{1/2}. \tag{24}$$

We have $\sum_{\mathbf{p}\in\Lambda^*} C_{\mathbf{p}} = -2\langle H\rangle + \lambda|\Lambda|$, which can be bounded from above using the following lower bound on the Hamiltonian:

$$H \geq -\frac{|\Lambda|}{4}\big[d(d+1) + 4\lambda^2\big]^{1/2} + \frac{1}{2}\lambda|\Lambda|. \tag{25}$$

This inequality follows from the fact that the lowest eigenvalue of

$$-\frac{1}{2} S^1_{\mathbf{x}} \sum_{i=1}^{2d} S^1_{\mathbf{y}_i} - \frac{1}{2} S^2_{\mathbf{x}} \sum_{i=1}^{2d} S^2_{\mathbf{y}_i} + \lambda S^3_{\mathbf{x}} \tag{26}$$

is given by $-\frac{1}{4}[d(d+1) + 4\lambda^2]^{1/2}$. This can be shown exactly in the same way as [9, Theorem C.1]. Since the Hamiltonian H can be written as a sum of terms like (26), with $\mathbf{y}_i$ the nearest neighbors of $\mathbf{x}$, we get from this fact the lower bound (25).

With the aid of the sum rule

$$\sum_{\mathbf{p}\in\Lambda^*} \langle \widetilde{S}^1_{\mathbf{p}} \widetilde{S}^1_{-\mathbf{p}} + \widetilde{S}^2_{\mathbf{p}} \widetilde{S}^2_{-\mathbf{p}} \rangle = \frac{|\Lambda|}{2}$$

(which follows from $(S^1)^2 = (S^2)^2 = 1/4$), we obtain from (24) and (25) the following lower bound in the thermodynamic limit:

$$\lim_{\Lambda\to\infty} \frac{1}{|\Lambda|} \langle \widetilde{S}^1_{\mathbf{0}} \widetilde{S}^1_{\mathbf{0}} + \widetilde{S}^2_{\mathbf{0}} \widetilde{S}^2_{\mathbf{0}} \rangle \geq \frac{1}{2} - \frac{1}{2} \left(\frac{1}{2} \left[d(d+1) + 4\lambda^2 \right]^{1/2} c_d \right)^{1/2} - \frac{1}{\beta} c_d, \tag{27}$$

with c_d given by

$$c_d = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} d\mathbf{p} \frac{1}{E_{\mathbf{p}}}. \tag{28}$$

This is our final result. Note that c_d is finite for $d \geq 3$. Hence the right side of (27) is positive, for large enough β, as long as

$$\lambda^2 < \frac{1}{c_d^2} - \frac{d(d+1)}{4}.$$

In $d = 3$, $c_3 \approx 0.505$ [9], and hence this condition is fulfilled for $\lambda \lesssim 0.960$. In [9] it was also shown that dc_d is monotone decreasing in d, which implies a similar result for all $d > 3$.

The connection with BEC is as follows. Since H is real, also $\gamma(\mathbf{x}, \mathbf{y})$ is real and we have

$$\gamma(\mathbf{x}, \mathbf{y}) = \langle S^+_{\mathbf{x}} S^-_{\mathbf{y}} \rangle = \langle S^1_{\mathbf{x}} S^1_{\mathbf{y}} + S^2_{\mathbf{x}} S^2_{\mathbf{y}} \rangle.$$

Hence, if $\varphi_0 = |\Lambda|^{-1/2}$ denotes the constant function,

$$\langle \varphi_0 | \gamma | \varphi_0 \rangle = \langle \widetilde{S}^1_{\mathbf{0}} \widetilde{S}^1_{\mathbf{0}} + \widetilde{S}^2_{\mathbf{0}} \widetilde{S}^2_{\mathbf{0}} \rangle,$$

and thus the bound (27) implies that the largest eigenvalue of $\gamma(\mathbf{x}, \mathbf{y})$ is bounded from below by the right side of (27) times $|\Lambda|$. In addition one can show that the infrared bounds imply that there is at most *one* large eigenvalue (of the order $|\Lambda|$), and that the corresponding eigenvector (the 'condensate wave function') is strictly constant in the thermodynamic limit [2]. The constancy of the condensate wave function is surprising and is not expected to hold for densities different from $\frac{1}{2}$, where particle-hole symmetry is absent. In contrast to the condensate wave function the particle density shows the staggering of the periodic potential [2, Theorem 3]. It also contrasts with the situation for zero interparticle interaction, as discussed at the end of this paper.

In the BEC phase there is *no gap* for adding particles beyond half filling (in the thermodynamic limit): The ground state energy, E_k, for $\frac{1}{2}|\Lambda| + k$ particles satisfies

$$0 \leq E_k - E_0 \leq \frac{(\text{const.})}{|\Lambda|} \tag{29}$$

(with a constant that depends on k but not on $|\Lambda|$.) The proof of (29) is by a variational calculation, with a trial state of the form $(\widetilde{S}^+_{\mathbf{0}})^k|0\rangle$, where $|0\rangle$ denotes the absolute ground state, i.e., the ground state for half filling. (This is the unique ground state of the Hamiltonian, as can be shown using reflection positivity. See Appendix A in [2].) Also, in the thermodynamic limit, the energy per site for a given density, $e(\varrho)$, satisfies

$$e(\varrho) - e\left(\frac{1}{2}\right) \leq \text{const.}\left(\varrho - \frac{1}{2}\right)^2. \tag{30}$$

Thus there is no cusp at $\varrho = 1/2$. To show this, one takes a trial state of the form

$$|\psi_{\mathbf{y}}\rangle = e^{\mathrm{i}\varepsilon \sum_{\mathbf{x}} S^2_{\mathbf{x}}}\left(S^1_{\mathbf{y}} + \frac{1}{2}\right)|0\rangle. \tag{31}$$

The motivation is the following: we take the ground state and first project onto a given direction of S^1 on some site $\mathbf{y}$. If there is long-range order, this should imply that essentially all the spins point in this direction now. Then we rotate slightly around the S^2-axis. The particle number should then go up by $\varepsilon|\Lambda|$, but the energy only by $\varepsilon^2|\Lambda|$. We refer to [2, Sect. IV] for the details.

The absence of a gap in the case of BEC is not surprising, since a gap is characteristic for a Mott insulator state. We show the occurrence of a gap, for large enough λ, in the next section.

4 Absence of BEC and Mott Insulator Phase

The main results of this section are the following: If either

- $\lambda \geq 0$ and $T > d/(2\ln 2)$, or
- $T \geq 0$ and $\lambda \geq 0$ such that $\lambda + |e(\lambda)| > d$, with $e(\lambda) =$ ground state energy per site,

then there is exponential decay of correlations:

$$\gamma(\mathbf{x}, \mathbf{y}) \leq (\text{const.}) \exp(-\kappa|\mathbf{x} - \mathbf{y}|) \tag{32}$$

with $\kappa > 0$. Moreover, for $T = 0$, the ground state energy in a sector of fixed particle number $N = \frac{1}{2}|\Lambda| + k$, denoted by E_k, satisfies

$$E_k + E_{-k} - 2E_0 \geq (\lambda + |e(\lambda)| - d)|k|. \tag{33}$$

I.e., for large enough λ the chemical potential has a jump at half filling.

The derivation of these two properties is based on a path integral representation of the equilibrium state at temperature T, and of the ground state which is obtained in the limit $T \to \infty$. The analysis starts from the observation that the density operator $e^{-\beta H}$ has non-negative matrix elements in the basis in which $\{S^3_{\mathbf{x}}\}$ are diagonal, i.e.

of states with specified particle occupation numbers. It is convenient to focus on the dynamics of the 'quasi-particles' which are defined so that the presence of one at a site $\mathbf{x}$ signifies a deviation there from the occupation state which minimizes the potential-energy. Since the Hamiltonian is $H = H_0 + \lambda W$, with H_0 the hopping term in (3) and W the staggered field, we define the quasi-particle number operators $n_{\mathbf{x}}$ as:

$$n_{\mathbf{x}} = \frac{1}{2} + (-1)^{\mathbf{x}} S^3_{\mathbf{x}} = \begin{cases} a^\dagger_{\mathbf{x}} a_{\mathbf{x}}, & \text{for } \mathbf{x} \text{ even} \\ 1 - a^\dagger_{\mathbf{x}} a_{\mathbf{x}}, & \text{for } \mathbf{x} \text{ odd} \end{cases} . \tag{34}$$

Thus $n_{\mathbf{x}} = 1$ means presence of a particle if $\mathbf{x}$ is on the A sublattice (potential maximum) and absence if $\mathbf{x}$ is on the B sublattice (potential minimum).

The collection of the joint eigenstates of the occupation numbers, $\{|\{n_{\mathbf{x}}\}\rangle\}$, provides a convenient basis for the Hilbert space. The functional integral representation of $\langle\{n_{\mathbf{x}}\}| e^{-\beta(H_0+\lambda W)} |\{n_{\mathbf{x}}\}\rangle$ involves an integral over configurations of quasi-particle loops in a *space* $\times$ *time* for which the (imaginary) 'time' corresponds to a variable with period β. The fact that the integral is over a positive measure facilitates the applicability of statistical-mechanics intuition and tools. One finds that the quasi-particles are suppressed by the potential energy, but favored by the entropy, which enters this picture due to the presence of the hopping term in H. At large λ, the potential suppression causes localization: long 'quasi-particle' loops are rare, and the amplitude for long paths decays exponentially in the distance, both for paths which may occur spontaneously and for paths whose presence is forced through the insertion of sources, i.e., particle creation and annihilation operators. Localization is also caused by high temperature, since the requirement of periodicity implies that at any site which participates in a loop there should be at least two jumps during the short 'time' interval $[0, \beta)$ and the amplitude for even a single jump is small, of order β.

The path integral described above is obtained through the Dyson expansion

$$e^{t(A+B)} = e^{tA} \sum_{m \geq 0} \int_{0 \leq t_1 \leq t_2 \leq \cdots \leq t_m \leq t} B(t_m) \cdots B(t_1) dt_1 \cdots dt_m \tag{35}$$

for any matrices A and B and $t > 0$, with $B(t) = e^{-tA} B e^{tA}$. (The $m = 0$ term in the sum is interpreted here as 1.)

In evaluating the matrix elements of $e^{-\beta H} = e^{-\beta(H_0+\lambda W)}$, in the basis $\{|\{n_{\mathbf{x}}\}\rangle\}$, we note that W is diagonal and $\langle\{n_{\mathbf{x}}\}|H_0|\{n'_{\mathbf{x}}\}\rangle$ is non-zero only if the configurations $\{n_{\mathbf{x}}\}$ and $\{n'_{\mathbf{x}}\}$ differ at exactly one nearest neighbor pair of sites where the change corresponds to either a creation of a pair of quasi-particles or the annihilation of such a pair. I.e., the matrix elements are zero unless $n_{\mathbf{x}} = n'_{\mathbf{x}}$ for all $\mathbf{x}$ except for a nearest neighbor pair $\langle \mathbf{xy} \rangle$, where $n_{\mathbf{x}} = n_{\mathbf{y}}$, $n'_{\mathbf{x}} = n'_{\mathbf{y}}$, and $n_{\mathbf{x}} + n'_{\mathbf{x}} = 1$. In this case, the matrix element equals $-1/2$.

Introducing intermediate states, the partition function can thus be written as follows:

$$\begin{aligned}\operatorname{Tr} e^{-\beta H} = \sum_{m=0}^{\infty} \int_{0\le t_1\le t_2\le\cdots\le t_m\le\beta} \sum_{|\{n_{\mathbf{x}}^{(i)}\}\rangle, 1\le i\le m} \\ \times \exp\left(-\lambda \sum_{i=1}^{m} (t_i - t_{i-1}) \sum_{\mathbf{x}} n_{\mathbf{x}}^{(i)}\right) dt_1\cdots dt_m \\ \times (-1)^m \langle\{n_{\mathbf{x}}^{(1)}\}|H_0|\{n_{\mathbf{x}}^{(m)}\}\rangle \langle\{n_{\mathbf{x}}^{(m)}\}|H_0|\{n_{\mathbf{x}}^{(m-1)}\}\rangle \\ \times \langle\{n_{\mathbf{x}}^{(m-1)}\}|H_0|\{n_{\mathbf{x}}^{(m-2)}\}\rangle \cdots \langle\{n_{\mathbf{x}}^{(2)}\}|H_0||\{n_{\mathbf{x}}^{(1)}\}\rangle \end{aligned} \tag{36}$$

with the interpretation $t_0 = t_m - \beta$. Note that the factor in the last two lines of (36) equals $(1/2)^m$ if adjacent elements in the sequence of configurations $\{n_{\mathbf{x}}^{(i)}\}$ differ by exactly one quasi-particle pair, otherwise it is zero.

Expansions of this type are explained more fully in [1]. A compact way of writing (36) is:

$$\operatorname{Tr} e^{-\beta H} = \int v(d\omega) e^{-\lambda|\omega|}. \tag{37}$$

Here the 'path' ω stands for a set of disjoint oriented loops in the 'space-time' $\Lambda \times [0, \beta]$, with periodic boundary conditions in 'time'. Each ω is parametrized by a number of jumps, m, jumping times $0 \le t_1 \le t_2 \le \cdots \le t_m \le \beta$, and a sequence of configurations $\{n_{\mathbf{x}}^{(i)}\}$, which is determined by the initial configuration $\{n_{\mathbf{x}}^{(1)}\}$ plus a sequence of 'rungs' connecting nearest neighbor sites, depicting the creation or annihilation of a pair of neighboring quasi-particles (see Fig. 2). As in Feynman's picture of QED, it is convenient to regard such an event as a jump of the quasi-particle, at which its time-orientation is also reversed. The length of ω, denoted by $|\omega|$, is the sum of the vertical lengths of the loops. The measure $v(d\omega)$ is determined by (36); namely, for a given sequence of configurations $\{n_{\mathbf{x}}^{(i)}\}$, $1 \le i \le m$, the integration takes places over the times of the jumps, with a measure $(1/2)^m dt_1 \cdots dt_m$.

One may note that the measure $v(d\omega)$ corresponds to a Poisson process of random configurations of oriented 'rungs', linking neighboring sites at random times, and signifying either the creation or the annihilation of a pair of quasiparticles. The matrix element $\langle\{n_{\mathbf{x}}\}|e^{-\beta H}|\{n'_{\mathbf{x}}\}\rangle$ gets no contribution from rung configurations that are inconsistent, either internally or with the boundary conditions corresponding to the specified state vectors. A consistent configuration yields a family of non-overlapping loops which describe the motion of the quasi-particles in the 'space-time' $\Lambda \times [0, \beta)$. Each such configuration contributes with weight $e^{-\lambda|\omega|}$ to the above matrix element (another positive factor was absorbed in the measure $v(d\omega)$). One may note that long paths are suppressed in the integral (39) at a rate which increases with λ.

Likewise, for $\mathbf{x} \ne \mathbf{y}$, we can write

$$\operatorname{Tr} a_{\mathbf{x}}^{\dagger} a_{\mathbf{y}} e^{-\beta H} = \int_{\mathscr{A}(\mathbf{x},\mathbf{y})} v(d\omega) e^{-\lambda|\omega|}, \tag{38}$$

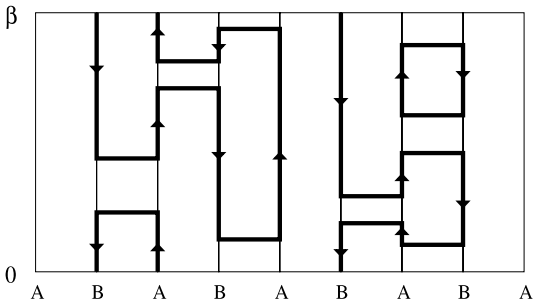

Fig. 2 Loop gas describing paths of quasi-particles for particle number $N = |\Lambda|/2 - 1$. A line on an A site means presence of a particle, while on a B site it means absence. The horizontal rungs correspond to hopping of a particle

where $\mathscr{A}^{(\mathbf{x},\mathbf{y})}$ denotes the set of all loops that, besides disjoint closed loops, contain one curve which avoids all the loops and connects $\mathbf{x}$ and $\mathbf{y}$ at time zero. The one-particle density matrix can thus be written

$$\gamma(\mathbf{x},\mathbf{y}) = \frac{\int_{\mathscr{A}^{(\mathbf{x},\mathbf{y})}} v(d\omega) e^{-\lambda|\omega|}}{\int v(d\omega) e^{-\lambda|\omega|}}. \tag{39}$$

For an upper bound, we can drop the condition in the numerator that the loops and the curve from $\mathbf{x}$ to $\mathbf{y}$ do not intersect. The resulting measure space is simply a Cartesian product of the measure space appearing in the denominator and the space of all curves, ζ, connecting $\mathbf{x}$ and $\mathbf{y}$, both at time 0. Denoting the latter by $\mathscr{B}(\mathbf{x},\mathbf{y})$, we thus get the upper bound

$$\gamma(\mathbf{x},\mathbf{y}) \leq \int_{\mathscr{B}(\mathbf{x},\mathbf{y})} v(d\zeta) e^{-\lambda|\zeta|}. \tag{40}$$

The integral over paths is convergent if either λ or T is small enough, and away from the convergence threshold the resulting amplitude decays exponentially. A natural random walk estimate, see [2, Lemma 4], leads to the claimed exponential bound provided

$$d\left(1 - e^{-\beta\lambda}\right) < \lambda. \tag{41}$$

This includes, in particular, the cases $T > d$ for any λ, and $\lambda > d$ for any T.

Exponential decay actually holds for the larger range of parameters where

$$d\left(1 - e^{-\beta(\lambda - f)}\right) < \lambda - f, \tag{42}$$

where $f = f(\beta,\lambda) = -(\beta|\Lambda|)^{-1} \ln \operatorname{Tr} e^{-\beta H}$ is the free energy per site. Note that $f < 0$. This condition can be obtained by a more elaborate estimate than the one used in obtaining (40) from (39), as shown in [2, Lemma 3]. The argument there uses reflection positivity of the measure $v(d\omega)$. Using simple bounds on f one can then obtain from (42) the conditions stated in the beginning of this section.

The proof of the energy gap is based on an estimate for the ratio $\frac{\mathrm{Tr}\,\mathscr{P}_k e^{-\beta H}}{\mathrm{Tr}\,\mathscr{P}_0 e^{-\beta H}}$ where $\mathscr{P}_k$ projects onto states in Fock space with particle number $N = \frac{1}{2}|\Lambda| + k$, expressing numerator and denominator in terms of path integrals. The integral for the numerator is over configurations ω with a non-trivial winding number k. Each such configuration includes a collection of 'non-contractible' loops with total length at least $\beta|k|$. An estimate of the relative weight of such loops yields the bound

$$\frac{\mathrm{Tr}\,\mathscr{P}_k e^{-\beta H}}{\mathrm{Tr}\,\mathscr{P}_0 e^{-\beta H}} \leq (\text{const.})(|\Lambda|/|k|)^{|k|}\left(e^{1-(\text{const.})\beta}\right)^{|k|} \tag{43}$$

which gives for $\beta \to \infty$

$$E_k - E_0 \geq (\text{const.})|k| \tag{44}$$

independently of $|\Lambda|$. We refer to [2] for details.

5 The Non-interacting Gas

The interparticle interaction is essential for the existence of a Mott insulator phase for large λ. In case of absence of the hard-core interaction, there is BEC for any density and any λ at low enough temperature (for $d \geq 3$). To see this, we have to calculate the spectrum of the one-particle Hamiltonian $-\frac{1}{2}\Delta + V(\mathbf{x})$, where Δ denotes the discrete Laplacian and $V(\mathbf{x}) = \lambda(-1)^{\mathbf{x}}$. The spectrum can be easily obtained by noting that V anti-commutes with the off-diagonal part of the Laplacian, i.e., $\{V, \Delta + 2d\} = 0$. Hence

$$\left(-\frac{1}{2}\Delta - d + V(\mathbf{x})\right)^2 = \left(-\frac{1}{2}\Delta - d\right)^2 + \lambda^2, \tag{45}$$

so the spectrum is given by

$$d \pm \sqrt{\left(\sum_i \cos p_i\right)^2 + \lambda^2}, \tag{46}$$

where $\mathbf{p} \in \Lambda^*$. In particular, $E(\mathbf{p}) - E(0) \sim \frac{1}{2}d(d^2 + \lambda^2)^{-1/2}|\mathbf{p}|^2$ for small $|\mathbf{p}|$, and hence there is BEC for low enough temperature. Note that the condensate wave function is of course *not* constant in this case, but rather given by the eigenfunction corresponding to the lowest eigenvalue of $-\frac{1}{2}\Delta + \lambda(-1)^{\mathbf{x}}$.

6 Conclusion

In this paper a lattice model is studied, which is similar to the usual Bose-Hubbard model and which describes the transition between Bose-Einstein condensation and a Mott insulator state as the strength λ of an optical lattice potential is increased. While the model is not soluble in the usual sense, it is possible to prove rigorously all the essential features that are observed experimentally. These include the existence of BEC for small λ and its suppression for large λ, which is a localization phenomenon depending heavily on the fact that the Bose particles interact with each other. The Mott insulator regime is characterized by a gap in the chemical potential, which does not exist in the BEC phase and for which the interaction is also essential. It is possible to derive bounds on the critical λ as a function of temperature.

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Random Walks in Random Environments in the Perturbative Regime

Ofer Zeitouni

Abstract We review some recent results concerning motion in random media satisfying an appropriate isotropy condition, in the perturbative regime in dimension $d \geq 3$.

1 Introduction

This talk reports on joint work with E. Bolthausen [1], as well as earlier joint work with A.-S. Sznitman [7]. We consider random walks in random environments on $\mathbb{Z}^d$, $d \geq 3$, when the environment is a small perturbation of the fixed environment corresponding to simple random walk. More precisely, let $\mathscr{P}$ be the set of probability distributions on $\mathbb{Z}^d$, charging only neighbors of 0. If $\varepsilon \in (0, 1/2d)$, we set, with $\{e_i\}_{i=1}^d$ denoting the standard basis of $\mathbb{R}^d$,

$$\mathscr{P}_\varepsilon \stackrel{\text{def}}{=} \left\{ q \in \mathscr{P} : \left| q(\pm e_i) - \frac{1}{2d} \right| \leq \varepsilon, \ \forall i \right\}. \tag{1}$$

$\Omega \stackrel{\text{def}}{=} \mathscr{P}^{\mathbb{Z}^d}$ is equipped with the natural product σ-field $\mathscr{F}$. We call an element $\omega \in \Omega$ a *random environment*. For $\omega \in \Omega$, and $x \in \mathbb{Z}^d$, we consider the transition probabilities $p_\omega(x, y) \stackrel{\text{def}}{=} \omega_x(y - x)$, if $|x - y| = 1$, and $p_\omega(x, y) = 0$ otherwise, and construct the random walk in random environment (RWRE) $\{X_n\}_{n \geq 0}$ with initial position $x \in \mathbb{Z}^d$ which is, given the environment ω, the Markov chain with $X_0 = x$ and transition probabilities

$$P_{\omega,x}(X_{n+1} = y | X_n = z) = \omega_z(y - z).$$

Ofer Zeitouni
Faculty of Mathematics, Weizmann Institute, Rehovot, Israel and School of Mathematics, University of Minnesota, Minneapolis, USA, e-mail: zeitouni@math.umn.edu

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We are mainly interested in the case of a *random* ω. Given a probability measure μ on $\mathscr{P}$, we consider the product measure $\mathbb{P}_\mu \stackrel{\text{def}}{=} \mu^{\otimes \mathbb{Z}^d}$ on $(\Omega, \mathscr{F})$. We usually drop the index μ in $\mathbb{P}_\mu$. In all that follows we make the following basic assumption.

Isotropy Condition *μ is invariant under lattice isometries, i.e. $\mu f^{-1} = \mu$ for any orthogonal mapping f which leaves $\mathbb{Z}^d$ invariant, and $\mu(\mathscr{P}_\varepsilon) = 1$ for some $\varepsilon \in (0, 1/2d)$ which will be specified later.*

The model of RWRE has been studied extensively. We refer to [6] and [8] for recent surveys. A major open problem is the determination, for $d > 1$, of laws of large numbers and central limit theorems in full generality (the latter, both under the *quenched* measure, i.e. for $\mathbb{P}_\mu$-almost every ω, and under the *annealed* measure $\mathbb{P}_\mu \otimes P_{x,\omega}$). Although much progress has been reported in recent years ([2, 4, 5]), a full understanding of the model has not yet been achieved.

In view of the above state of affairs, attempts have been made to understand the perturbative behavior of the RWRE, that is the behavior of the RWRE when μ is supported on $\mathscr{P}_\varepsilon$ and ε is small. The first to consider such a perturbative regime were [3], who introduced the Isotropy Condition and showed that in dimension $d \geq 3$, for small enough ε a quenched CLT holds.[1] Unfortunately, the multiscale proof in [3] is rather difficult, and challenging to follow. This in turns prompted the derivation, in [7], of an alternative multiscale approach, in the context of diffusions in random environments. The main result of [7] can be described as follows. Consider a diffusion with random coefficients on $\mathbb{R}^d$,

$$dX_t = b(X_t, \omega)dt + \sigma(X_t, \omega)dW_t,$$

with $W_\cdot$ a d-dimensional Brownian motion and $a(x, \omega) = \sigma(x, \omega)\sigma^T(x, \omega)$. Assume the local characteristics a, b are uniformly Lipshitz in the space variable, stationary, and of finite range dependence, and further satisfy an isotropy condition of the type described above. One then has the following.

Theorem 1 ([7]). *($d \geq 3$) There is $\eta_0 > 0$, such that when*

$$|a(x, \omega) - I| \leq \eta_0, \qquad |b(x, \omega)| \leq \eta_0, \quad \text{for all } x \in \mathbb{R}^d, \omega \in \Omega, \tag{2}$$

then for P-a.e., ω

$$\frac{1}{\sqrt{t}} X_{\cdot t} \text{ converges in } P_{0,\omega}\text{-law as } t \to \infty, \text{ to a Brownian motion}$$
$$\text{on } \mathbb{R}^d \text{ with deterministic variance } \sigma^2 > 0, \tag{3}$$
$$\text{for all } x \in \mathbb{R}^d, \ P_{x,\omega}\text{-a.s.}, \ \lim_{t\to\infty} |X_t| = \infty. \tag{4}$$

One expects that the approach of [7] could apply to the discrete setup, as well.

[1] As the examples in [2] demonstrate, for every $d \geq 7$ and $\varepsilon > 0$ there are measures μ supported on $\mathscr{P}_\varepsilon$, with $\mathbb{E}_\mu[\sum_{i=1}^d e_i(q(e_i) - q(-e_i))] = 0$, such that $X_n/n \to_{n\to\infty} v \neq 0$, $\mathbb{P}_\mu$-a.s. One of the goals of the Isotropy Condition is to prevent such situations from occurring.

The proof of Theorem 1 is based on a multiscale analysis that includes the appropriate smoothing (with respect to Hölder norms) of the transition density of the diffusion, together with controlling exit measures from boxes, and in particular their large deviations. The latter is a crucial part of the control of exit time from traps. A naturally related question is whether focusing on exit measures from balls, i.e. not considering at all the time to exit, can simplify the analysis on the one hand, and provide sharp (local) estimates on exit on the other. The affirmative answer to these questions in provided in [1], which we summarize in the next section. In contrast with [7], we focus on two ingredients. The first is a propagation of the variational distance between the exit laws of the RWRE from balls and those of simple random walk (which distance remains small but does not decrease as the scale increases). The second is the propagation of the variation distance between the convolution of the exit law of the RWRE with the exit law of a simple random walk from a ball of (random) radius, and the corresponding convolution of the exit law of simple random walk with the same smoothing, which distance decreases to zero as scale increases.

2 Local Limits for Exit Measures

Throughout, for $x \in \mathbb{R}^d$, $|x|$ is the Euclidean norm. If $L > 0$, we write $V_L \stackrel{\text{def}}{=} \{x \in \mathbb{Z}^d : |x| \le L\}$, and for $x \in \mathbb{Z}^d$, $V_L(x) \stackrel{\text{def}}{=} x + V_L$.

If F, G are functions $\mathbb{Z}^d \times \mathbb{Z}^d \to \mathbb{R}$ we write FG for the (matrix) product: $FG(x, y) \stackrel{\text{def}}{=} \sum_u F(x, u)G(u, y)$, provided the right hand side is absolutely summable. We interpret F also as a kernel, operating from the left on functions $f : \mathbb{Z}^d \to \mathbb{R}$, by $Ff(x) \stackrel{\text{def}}{=} \sum_y F(x, y)f(y)$. For a function $f : \mathbb{Z}^d \to \mathbb{R}$, $\|f\|_1 \stackrel{\text{def}}{=} \sum_x |f(x)|$. If F is a kernel then, we write

$$\|F\|_1 \stackrel{\text{def}}{=} \sup_x \|F(x, \cdot)\|_1. \tag{5}$$

For $V \subset \mathbb{Z}^d$, we use $\pi_V(x, \cdot)$ to denote the exit measure from V of simple random walk started from x, and use $\Pi_V(x, \cdot)$ for the analogous quantity for the RWRE. Fix once for all a probability density

$$\varphi : \mathbb{R}^+ \to \mathbb{R}^+,\ \varphi \in C^\infty,\ \text{support}(\varphi) = [1, 2]. \tag{6}$$

If $m > 0$, the rescaled density is defined by $\varphi_m(t) \stackrel{\text{def}}{=} (1/m)\varphi(t/m)$. We then let $\hat{\pi}_{\Psi_m}(x, \cdot)$ denote the exit measure of simple random walk started at x from a ball with random radius R distributed according to φ_m.

For $x \in \mathbb{Z}^d$, $t \in \mathbb{R}$, and $L > 0$, we define the random variables

$$D_{L,t}(x) \stackrel{\text{def}}{=} \left\| \left(\left[\Pi_{V_L(x)} - \pi_{V_L(x)} \right] \hat{\pi}_{\Psi_t} \right)(x, \cdot) \right\|_1, \tag{7}$$

$$D_{L,0}(x) \stackrel{\text{def}}{=} \left\| \Pi_{V_L(x)}(x, \cdot) - \pi_{V_L(x)}(x, \cdot) \right\|_1, \tag{8}$$

and with $\delta > 0$, we set

$$b(L,t,\delta) \stackrel{\text{def}}{=} \mathbb{P}\big(\big\{(\log L)^{-9} < D_{L,t}(0)\big\} \cup \{D_{L,0}(0) > \delta\}\big).$$

The following theorem is the main result of [1]. It provides a local limit theorem for the exit law.

Theorem 2 ([1]). *($d \geq 3$) There exists $\varepsilon_0 > 0$, such that if the Isotropy Condition is satisfied with $\varepsilon \leq \varepsilon_0$, then for any $\delta > 0$, and for any integer $r \geq 0$,*

$$\lim_{t\to\infty} \limsup_{L\to\infty} L^r b(L, \Psi_t, \delta) = 0.$$

Further, the RWRE X_n is transient, that is

$$\text{for all } x \in \mathbb{Z}^d,\ P_{x,\omega}\text{-a.s.},\ \lim_{n\to\infty} |X_n| = \infty.$$

The Borel-Cantelli lemma implies that under the conditions of Theorem 2,

$$\limsup_{L\to\infty} D_{L,\Psi_t}(0) \leq c_t, \quad \mathbb{P}_\mu\text{-a.s.},$$

where c_t is a (random) constant such that $c_t \to_{t\to\infty} 0$, a.s.

We remark that the rate of decay of probabilities in Theorem 2 is not expected to be optimal, rather it is dictated by the multiscale-scale scheme employed in the proof. We also remark that proving an analogue of the local limit result for the exit measure in Theorem 2 for dimension $d = 2$ is an open problem; the method of proof employed both in [7] and [1] uses the transience of simple random walk (and the finiteness of associated Green functions) in a crucial way.

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Appendix: Complete List of Abstracts

YRS and XV ICMP

1 Young Researchers Symposium Plenary Lectures

1.0.1 Dynamics of Quasiperiodic Cocycles and the Spectrum of the Almost Mathieu Operator

Artur Avila
CNRS
artur@math.sunysb.edu

The almost Mathieu operator is the operator $H : l^2(\mathbb{Z}) \to l^2(\mathbb{Z})$,

$$(Hu)_n = u_{n+1} + u_{n-1} + 2\lambda \cos 2\pi(\theta + n\alpha),$$

where λ (the coupling), α (the frequency) and θ (the phase) are parameters. Originally introduced and studied in the physics literature, it turned out to also give rise to a rich mathematical theory, where algebra, analysis and dynamical systems interact. We will discuss several conjectures that have focused the developments since 1980, emphasizing the connection with dynamical systems.

1.0.2 Magic in Superstring Amplitudes

Nathan Jacob Berkovits
UNESP, São Paulo
nberkovi@ift.unesp.br

In this talk, a chronological review will be given of scattering amplitudes in superstring theory and their remarkable properties. I will start with the Veneziano amplitude of 1968 which led to bosonic string theory, and subsequent developments in the 70's which led to supersymmetry and superstring theory. I will then discuss the amplitude calculations of Green and Schwarz in the 80's which led to aspirations of

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unifying the forces, and the non-perturbative dualities discovered in the 90's which led to the M-theory conjecture. Finally, I will discuss recent developments using a covariant description of the superstring in which some of these magical properties are easier to study.

1.0.3 The Instructive History of Quantum Groups

Ludwig Faddeev
Petersburg Department of Steklov Institute of Mathematics
faddeev@euclid.pdmi.ras.ru

I shall try to use this example to show, how concrete problems in Mathematical Physics (here quantum spin chains) can lead to new construction in pure mathematics.

1.0.4 Scaling Limit of Two-Dimensional Critical Percolation

Charles M. Newman
Courant Institute, NYU
newman@courant.nyu.edu

We introduce and discuss the continuum nonsimple loop process (joint work with F. Camia). This process, which describes the full scaling limit of 2D critical percolation, consists of countably many noncrossing nonsimple loops in the plane on all spatial scales; it is based on the Schramm Loewner Evolution (with parameter 6) and extends the work of Schramm and Smirnov on the percolation scaling limit. If time permits, we will introduce some ideas associated with the further extension to scaling limits of "near-critical" percolation (joint work with F. Camia and L.R. Fontes).

1.0.5 Topics in Dynamics and Physics

David Ruelle
IHES
ruelle@ihes.fr

The study of dynamics (i.e., time evolutions) is central to physics. I shall discuss several questions of mathematical physics connected with differentiable dynamical systems and related, as it happens, to the ideas of Henri Poincare. I shall go from chaos in turbulence and celestial mechanics to the symbolic dynamics of horseshoes and other hyperbolic dynamical systems, to the dynamics underlying nonequilibrium statistical mechanics.

1.0.6 Quantum Dynamics in a Random Environment

Thomas Spencer
IAS, Princeton
spencer@ias.edu

The first part of this talk will review results and conjectures on the quantum and classical dynamics of a particle moving in a random environment. In general, classical and quantum dynamics are qualitatively different. We review a particular network model studied by J. Cardy and others for which classical and quantum motion are equivalent and compare it to the mirror model.

The second part of the talk will describe a supersymmetric approach to quantum evolution generated by band random matrices. The supersymmetric approach converts time evolution into a problem in which the randomness is integrated out. This produces a statistical mechanics model with hyperbolic symmetry. One is lead to study of determinants and Greens functions of nonuniformly elliptic PDE.

1.0.7 Geometry of Low Dimensional Manifolds

Gang Tian
Princeton
tian@Math.Princeton.edu

In this talk, I will first discuss Perelman's work on proving the Poincare conjecture and the geometrization of 3-manifolds. Perelman's work is based on Hamilton's fundamental work on Ricci flow. In the end, I will discuss recent progress on geometry and analysis of 4-manifolds and propose some problems.

1.0.8 Gauge Theory and the Geometric Langlands Program

Edward Witten
IAS, Princeton
witten@ias.edu

I will explain how electric-magnetic duality in gauge theory can be used to understand a problem in algebraic geometry known as the geometric Langlands program.

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2.0.1 Mathematical Developments Around the Ginzburg-Landau Model in 3D Program

Jean Bourgain
IAS, Princeton
bourgain@ias.edu

We are discussing the 3D Ginzburg Landau functional without magnetic field in the London limit,which is the 3D counterpart of the work of Bethuel-Brezis-Helein.In particular the role of the minimal connection in the evaluation of the Ginzburg-Landau energy is explained and optimal regularity properties of the minimizers stated. A key role is played by certain novel Hodge decompositions at the critical Sobolev index.

2.0.2 The Riemann-Hilbert Problem: Applications

Percy Deift
Courant Institute, NYU
deift@courant.nyu.edu

In this talk the speaker will describe the application of Riemann-Hilbert techniques to a variety of problems in mathematics and mathematical physics. Algebraic and analytical applications will be discussed. The nonlinear steepest descent method plays a key role.

2.0.3 Fluctuations and Large Deviations in Non-equilibrium Systems

Bernard Derrida
ENS, Paris
derrida@lps.ens.fr

Systems in contact with two heat baths at unequal temperatures or two reservoirs of particles at unequal densities reach non-equilibrium steady states. For some simple models, one can calculate exactly the large deviation functions of the density profiles or of the current in such steady states.

These simple examples show that non-equilibrium systems have a number of properties which contrast with equilibrium systems: phase transitions in one dimension, non local free energy functional, violation of the Einstein relation between the compressibility and the density fluctuation, non-Gaussian density fluctuations.
In collaboration with T. Bodineau, J.L. Lebowitz, E.R. Speer.

2.0.4 Hamiltonian Perturbations of Hyperbolic PDE's: from Classification of Equations to Properties of Solutions

Boris Dubrovin
SISSA, Trieste
dubrovin@sissa.it

The talk will deal with the classification of Hamiltonian perturbations of hyperbolic PDEs with one spatial dimension and with the comparative study of their singularities.

2.0.5 Spontaneous Replica Symmetry Breaking in the Mean Field Spin Glass Model

Francesco Guerra
Universita Roma 1 "La Sapienza"
Francesco.Guerra@roma1.infn.it

We give a complete review about recent methods and results in the mean field spin glass theory. In particular, we show how it has been possible to establish the rigorous validity of the Parisi representation for the free energy in the infinite volume limit. The origin of the Parisi functional order parameter is explained in the frame of Derrida-Ruelle probability cascades. Finally, we conclude with an outlook on possible future developments.

2.0.6 Spectral Properties of Quasi-Periodic Schrödinger Operators: Treating Small Denominators without KAM

Svetlana Jitomirskaya
UC-Irvine
szhitomi@math.uci.edu

Two classical small divisor problems arise in the study of spectral properties of quasiperiodic Schroedinger operators, one related to Floquet reducibility (for low couplings of the potential term), and the other related to localization (for high couplings). Both have been traditionally attacked by sophisticated KAM-type methods.

In this talk I will discuss more recent non-KAM based methods for both localization and reducibility, that are significantly simpler and lead, where applicable, to stronger results. In particular they usually lead to so-called nonperturbative (i.e. uniform in the Diophantine frequency) estimates on the coupling, and sometimes to the results covering the entire expected region of couplings.

I will discuss the recent joint work with A. Avila on nonperturbative reducibility, with various sharp spectral consequences in the low coupling regime, and review earlier results by J. Bourgain, M. Goldstein, W. Schlag, and the speaker, on nonperturbative localization.

2.0.7 Conformal Field Theory and Operator Algebras

Yasuyuki Kawahigashi
University of Tokyo
yasuyuki@ms.u-tokyo.ac.jp

Algebraic quantum field theory is an operator algebraic approach to quantum field theory and its main object is a family of operator algebras parameterized by spacetime regions, rather than Wightman fields. I will present recent progress on classification of conformal field theories within this approach.

Chiral, full and boundary conformal field theories are described in a unified framework and we present their complete classification for the case where the central charge is less than 1. In the chiral case, our classification list contains an example which does not seem to be known in other approaches to conformal field theory. Our tools are based on operator algebraic representation theory and are applications of the Jones theory of subfactors. Similar methods are also useful for operator algebraic studies of the Moonshine conjecture.

This is a joint work with Roberto Longo.

2.0.8 Random Schrödinger Operators, Localization and Delocalization, and all that

Abel Klein
UC, Irvine
aklein@math.uci.edu

In the widely accepted picture of the spectrum of a random Schrödinger operator in three or more dimensions, there is a transition from an *insulator region*, characterized by "localized states", to a very different *metallic region*, characterized by "extended states". The energy at which this *metal-insulator transition* occurs is called the *mobility edge*. The standard mathematical interpretation of this picture translates "localized states" as pure point spectrum with exponentially decaying eigenstates (Anderson localization) and "extended states" as absolutely continuous spectrum.

Forty some years have passed since Anderson's seminal article but our mathematical understanding of this picture is still unsatisfactory and one-sided: the occurrence of Anderson localization is by now well established, but with the exception of the special case of the Anderson model on the Bethe lattice, there are no mathematical results on the existence of continuous spectrum and a metal-insulator transition.

In this lecture I will first review localization, including the recent proofs of localization for the Bernoulli-Anderson Hamiltonian (Bourgain and Kenig) and for the Poisson Hamiltonian (Germinet, Hislop and Klein).

I will then present an approach to the metal-insulator transition based on dynamical (i.e., transport) instead of spectral properties (Germinet and Klein). Here transport refers to the rate of growth, with respect to time, of moments of a wave packet initially localized both in space and energy. The *region of dynamical localization* is

defined to be the spectral region where the random Schrödinger operator exhibits strong dynamical localization, and hence no transport. The *region of dynamical delocalization* is the spectral region with nontrivial transport. There is a natural definition of a *dynamical metal-insulator transition* and of a *dynamical mobility edge*. We proved a structural result on the dynamics of Anderson-type random operators: at a given energy there is either dynamical localization or dynamical delocalization with a nonzero minimal rate of transport. The region of dynamical localization turns out to be the analogue for random operators of Dobrushin-Shlosman's region of complete analyticity for classical spin systems, and may be called the *region of complete localization*.

I will close with the proof of the occurrence of this *dynamical metal-insulator transition* in random Landau Hamiltonians (Germinet, Schenker and Klein). More precisely, we show the existence of dynamical delocalization for random Landau Hamiltonians near each Landau level, which combined with the known dynamical localization at the edges of each disordered-broadened Landau band, implies the existence of at least one dynamical mobility edge in each Landau band.

2.0.9 Perelman's Work on the Geometrization Conjecture

Bruce Kleiner
Yale
bruce.kleiner@yale.edu

The lecture will discuss the Ricci flow approach to Geometrization.

2.0.10 Trying to Characterize Robust and Generic Dynamics

Enrique Ramiro Pujals
IMPA, Rio de Janeiro
enrique@impa.br

If we consider that the mathematical formulation of natural phenomena always involves simplifications of the physical laws, real significance of a model may be accorded only to those properties that are robust under perturbations. In loose terms, robustness means that some main features of a dynamical system (an attractor, a given geometric configuration, or some form of recurrence, to name a few possibilities) are shared by all nearby systems.

In the talk, we will explain the structure related to the presence of robust phenomena and the universal mechanisms that lead to lack of robustness. Providing a conceptual framework, the goal is to show how this approach helps to describe "generic" dynamics in the space of all dynamical systems.

2.0.11 Cauchy Problem in General Relativity

Igor Rodnianski
Princeton
irod@Math.Princeton.edu

The talk will describe some of the classical and recent results on the Cauchy problem in General Relativity. Special focus will be on the problems concerning existence of a Cauchy development, break-down criteria for general large data solutions, stability questions, and connections to the nonlinear hyperbolic equations.

2.0.12 Survey of Recent Mathematical Progress in the Understanding of Critical 2d Systems

Wendelin Werner
Université Paris-Sud
wendelin.werner@math.u-psud.fr

In this talk, I will try to survey some aspects of the recent progress in the mathematical understanding of random and conformally invariant two-dimensional structures. I will in particular describe work by or in collaboration with Greg Lawler, Oded Schramm, Scott Sheffield, Stas Smirnov, and I will mention and define SLE processes, Brownian loop-soups, Gaussian Free Fields. These conformally invariant structures are supposed to (and in some cases it is proved) to appear as scaling limits of two-dimensional critical models from statistical physics, and to be therefore rather directly related to conformal field theory.

2.0.13 Random Methods in Quantum Information Theory

Andreas Winter
University of Bristol
a.j.winter@bristol.ac.uk

The probabilistic method—or "random coding" in information theory—is the most powerful tool to construct efficient information processing protocols. I will review the status of random coding in quantum information theory in the light of recent progress in understanding random channel codes and entanglement distillation procedures. Applications include an operational interpretation of quantum conditional entropy ("negative information"), an approach to the foundations of statistical mechanics based on entanglement and the existence of exotic, highly entangled yet barely correlated states.

2.0.14 Gauge Fields, Strings and Integrable Systems

Konstantin Zarembo
Uppsala University
Konstantin.Zarembo@teorfys.uu.se

The discovery of the holographic duality made it clear that there is a tight relationship between gauge fields and strings. Quite unexpectedly, this relationship involves close ties to quantum spin chains and integrable systems. I will review various aspects of the gauge/string duality, and will explain how integrability arises in gauge and string theories.

3 XV International Congress on Mathematical Physics Specialized Sessions

3.1 Condensed Matter Physics

Organizer J.P. Solovej (Copenhagen)

3.1.1 Rigorous Construction of Luttinger Liquids Through Ward Identities

Giuseppe Benfatto
Università di Roma "Tor Vergata"
benfatto@mat.uniroma2.it

There are up to now two different ways to prove the key property on which our Luttinger liquid rigorous construction rests, the vanishing of the leading part of the Beta function.

The first one was developed in the last years and is based in an essential way on the exact Mattis-Lieb solution of the Luttinger model.

More recently, we found a new proof, based on the Ward identities obtained by a chiral local gauge transformation, applied to a Luttinger model with ultraviolet and infrared cutoffs. This is an old approach in the physical literature, but its implementation in an RG scheme is not trivial at all, because the ultraviolet and infrared cutoffs destroy local Gauge invariance and produce "correction terms" with respect to the formal Ward identities. We discover however a new set of identities, called "Correction Identities", relating the corrections to the Schwinger functions. By combining Ward and Correction identities with a Dyson equation, the vanishing of the Beta function follows, so that the infrared cutoff can be removed.

As a byproduct, even the ultraviolet cutoff can be removed, after a suitable ultraviolet renormalization, so that a Quantum Field Theory corresponding to the Thirring model is constructed, showing the phenomenon of Chiral anomaly.

3.1.2 Edge and Bulk Currents in the Integer Quantum Hall Effect

Jeffrey Schenker
Institute for Advanced Study
jeffrey@ias.edu

Two apparently different conductances σ_{Bulk} and σ_{Edge} have been used to explain the integer quantum Hall effect, depending on whether the currents in the sample are ascribed to the bulk or the edge. The bulk conductance σ_{Bulk}, as expressed through a linear response formula, is well defined when the Fermi energy falls in a mobility gap, that is a band of localized states. However, the edge conductance σ_{Edge}, expressed as the derivative of the steady state edge current with respect to the Fermi energy, is ill defined unless the Fermi energy falls in true gap. A physically suitable expression for σ_{Edge} can be obtained from a modified formula involving either (1) a truncated trace and a correction term or (2) time averaging. With this modified expression the equality $\sigma_{Edge} = \sigma_{Bulk}$ is a theorem, as expected from heuristic arguments. (Joint work with A. Elgart and G.M. Graf)

3.1.3 Quantum Phases of Cold Bosons in Optical Lattices

Jakob Yngvason
Universität Wien
yngvason@thor.thp.univie.ac.at

In recent years it has become possible to trap ultracold atoms and molecules in lattices generated by laser beams (optical lattices). By varying the experimentally tunable parameters transitions between various phases of the trapped gas, in particular between a Bose Einstein condensate and a Mott insulator phase, can be produced. The talk reviews these developments, and rigorous theoretical results on such transitions, obtained in collaboration with M. Aizenman, E.H. Lieb, R. Seiringer and J.P. Solovej, will be presented.

3.2 Dynamical Systems

Organizers W. de Mello (Rio de Janeiro), F. Ledrappier (Notre Dame)

3.2.1 Statistical Stability for Hénon Maps of Benedics-Carleson Type

Jose Ferreira Alves
University of Porto
jfalves@fc.up.pt

We consider the two-parameter family of Hénon maps in the plane $(x, y) \mapsto (1 - ax^2 + y, bx)$. Benedicks and Carleson proved that there is a positive Lebesgue measure set A of parameters (a, b) for which the corresponding Hénon map has a chaotic attractor. Subsequent work by Benedicks and Young showed that each of these attractors supports an SRB measure, i.e. a probability measure which describes the statistics of Lebesgue almost every point in a neighborhood of the attractor. Here we show that the SRB measures vary continuously in weak* topology with the parameters $(a, b) \in A$. This is a joint work with M. Carvalho and J.M. Freitas.

3.2.2 Entropy and the Localization of Eigenfunctions

Nalini Anantharaman
ENS-Lyon
Nalini.Anantharaman@umpa.ens-lyon.fr

We study the large eigenvalue limit for eigenfunctions of the Laplacian, on a compact negatively curved manifold. According to the Quantum Unique Ergodicity conjecture, eigenfunctions must become equidistributed in phase space, meaning that the Wigner transforms of eigenfunctions must converge weakly to the Liouville measure. We find a positive lower bound for the Kolmogorov-Sinai entropy of limits of these Wigner measures, which shows that eigenfunctions must be delocalized to a certain extent. Part of this work is joint with Stephane Nonnenmacher (CEA Saclay).

3.2.3 The Spectrum of the Almost Mathieu Operator in the Subcritical Regime

Artur Ávila
CNRS-Jussieu
artur@math.sunysb.edu

We discuss the almost Mathieu operator $H : l^2(\mathbb{Z}) \to l^2(\mathbb{Z})$, $(Hu)_n = u_{n+1} + u_{n-1} + 2\lambda \cos 2\pi(\theta + n\alpha)$, where $\lambda > 0$ (the coupling), $\alpha \in \mathbb{R} \setminus \mathbb{Q}$ (the frequency), and $\theta \in \mathbb{R}$ (the phase) are parameters. The nature of the spectral measures has been subject of several conjectures since 1980, when Aubry-André proposed the following picture:

1-Localization (point spectrum with exponentially decaying eigenfunctions) for the supercritical regime $\lambda > 1$,

2-Absolutely continuous spectrum for the subcritical regime $\lambda < 1$, both regimes being linked by Aubry duality.

Localization turns out to be very sensitive to arithmetics (and fails generically), so the description of the supercritical regime could only be proved in the "almost

every" sense. Whether something similar happened in the subcritical regime remained unclear. We will discuss recent progress towards the complete solution of this problem.

3.2.4 Hyperbolicity Through Entropy

Jerome Buzzi
École Polytechnique
buzzi@math.polytechnique.fr

We show how (robust) entropy assumptions yields (what we call) semi-uniform hyperbolic structures which allow the global analysis of some classes of smooth dynamical systems from the point of view of their complexity. These classes include coupled interval maps with positive entropy and models for surface diffeomorphisms.

3.2.5 Robust Cycles and Non-dominated Dynamics

Lorenzo J. Diaz
PUC – Rio de Janeiro
lodiaz@mat.puc-rio.br

The Newhouse's construction of C^2-surface diffeomorphisms having a hyperbolic sets with robust tangencies relies on the notion of thick hyperbolic set. These thick hyperbolic sets are the key for so-called coexistence phenomenon (existence of locally residual sets of diffeomorphisms having simultaneously infinitely many sinks and sources). These constructions are typically C^2. The goal of this talk is to discuss similar phenomena in higher dimensions and in the C^1-topology.

We first explain the generation of robust cycles in the C^1-topology and obtain some dynamical consequences from this fact. We also discuss the role of the robust cycles for generating robustly non-dominated dynamics and deduce some strong forms of the coexistence phenomenon from the lack of domination.

3.2.6 Hyperbolicity in One Dimensional Dynamics

Oleg Kozlovskiy
Warwick Mathematics Institute
oleg@maths.warwick.ac.uk

Recently together with W. Shen and S. van Strien we were able to prove dencity of hyperbolicity for all real one dimensional maps and also for a large class of one dimensional holomorphic maps. During the talk we will discuss these results together with other recent developments in the subject.

3.3 Equilibrium Statistical Mechanics

Organizer C.M. Newman (New York)

3.3.1 The Scaling Limit of (Near-)Critical 2d Percolation

Federico Camia
Vrije Universiteit Amsterdam
fede@few.vu.nl

The introduction of the random fractal curves described by Schramm-Loewner Evolutions (SLEs) has greatly deepened our understanding of the large-scale structure and fractal properties of certain two-dimensional lattice models whose continuum scaling limit is known or conjectured to be conformally invariant.

A particularly illuminating example is that of critical percolation, where the connection with SLE can be made rigorous and can be exploited to describe the scaling limit of the model in terms of the collection of all its interfaces.

In turn, this description can be used to analyze the scaling limit of near- critical percolation and related models. The emerging picture suggests that the conformal invariance typical of critical models is replaced by a more general type of invariance under conformal transformation.

In this talk I will describe joint work with C.M. Newman and with L.R. Fontes and C.M. Newman on the scaling limit of critical and near-critical percolation.

3.3.2 Short-Range Spin Glasses in a Magnetic Field

Daniel Stein[*+]
NYU
daniel.stein@nyu.edu

The thermodynamic behavior of short-range spin glasses in small magnetic fields and at low temperatures remains an open problem. Results elucidating the consequences of applying a magnetic field can provide a powerful tool in understanding the low-temperature behavior of realistic spin glasses, in particular the nature of their broken symmetry, phase diagram, and other fundamental thermodynamic information. I will discuss new techniques that have recently been developed to treat this problem, and present some preliminary results that clarify the effects of a magnetic field on short-range spin glasses.

[*]In collaboration with C.M. Newman, Courant Institute, New York University.
[+]Research supported by the U.S. National Science Foundation.

3.3.3 Relaxation Times of Kinetically Constrained Spin Models with Glassy Dynamics

Cristina Toninelli
Université Paris Sud—CNRS
Cristina.Toninelli@lpt.ens.fr

We discuss kinetically constrained spin models (KCSM), that is interacting particle systems with Glauber-like dynamics in which the creation/destruction of a particle can occur only if the configuration satisfies some local constraints. KCSM were introduced in physical literature to model liquid/glass transition. Numerical simulations show that, as density ρ is increased, they display an anomalously slow dynamics and glassy features including stretched exponential relaxation. We present a new probabilistic technique through which we determine the scaling with the system size of the relaxation time, τ, and we obtain upper and lower bounds for its dependence on ρ. On the one hand, we prove that τ diverges for some models faster than any power law of $1-\rho$ as $\rho \nearrow 1$. On the other hand, we establish exponential decay of spin-spin time auto-correlation functions for all the models in the ergodic regime. This excludes the stretched exponential relaxation conjectured from simulations, which is due to the rapid divergence of τ.

3.4 Non-equilibrium Statistical Mechanics

Organizers G. Jona-Lasinio (Rome), B. Nachtergaele (Davis)

3.4.1 Current Fluctuations in Boundary Driven Interacting Particle Systems

Claudio Landim
IMPA
landim@impa.br

We present a review of recent work on the statistical mechanics of non equilibrium processes based on the analysis of large deviations properties of microscopic systems. Stochastic lattice gases are non trivial models of such phenomena and can be studied rigorously providing a source of challenging mathematical problems. In this way, some principles of wide validity have been obtained leading to interesting physical consequences.

3.4.2 Fourier Law and Random Walks in Evolving Environments

Carlangelo Liverani
Università di Roma "Tor Vergata"
liverani@mat.uniroma2.it

Motivated by the problem of rigorously establishing the Fourier law for solids we introduce a simple toy model consisting of a spatially extended partially hyperbolic dynamical system. In turn such a model can be interpreted as a random walk in an evolving environment. Some rigorous results are obtained for the latter systems.

3.4.3 Asymptotics of Repeated Interaction Quantum Systems

Marco Merkli
McGill University
mmerkli@fields.utoronto.ca

A quantum system $\mathcal{S}$ interacts in a successive way with elements $\mathcal{E}$ of a chain of identical independent quantum subsystems. Each interaction lasts for a duration τ and is governed by a fixed coupling between $\mathcal{S}$ and $\mathcal{E}$. We show that the system, initially in any state close to a reference state, approaches a *repeated interaction asymptotic state* in the limit of large times. This state is τ-periodic in time and does not depend on the initial state. If the reference state is chosen so that $\mathcal{S}$ and $\mathcal{E}$ are individually in equilibrium at positive temperatures, then the repeated interaction asymptotic state satisfies an average second law of thermodynamics.

This is a collaboration with L. Bruneau and A. Joye.

3.4.4 Linear Response of Non-equilibrium Steady States for Open Quantum System

Claude-Alain Pillet
Université Toulon-Var
pillet@univ-tln.fr

I will present recent results with V. Jaksic and Y. Ogata on the linear response theory of thermally driven open quantum systems. These include

- A derivation of the Green-Kubo formulas and Onsager reciprocity relations in the abstract framework of nonequilibrium steady states (NESS).
- Two classes of realization of this framework: The scattering approach to locally interacting Fermi gases and the Liouvillean resonance approach to open systems.

These two classes of models are well suited for application to the physics of nanoscopic devices out of equilibrium. I will briefly discuss the connections with other

well known approaches (Weak coupling or master equation approach, Landauer-Buettiker scattering approach to independent electron systems, Keldysh formalism and Meir-Wingreen approach to locally interacting Fermions).

3.4.5 Derivation of the Gross-Pitaevski Equation for the Dynamics of Bose-Einstein Condensates

Benjamin Schlein
Harvard
schlein@math.harvard.edu

In this talk I am going to report on a recent result obtained in collaboration with L. Erdoes and H.-T. Yau. We consider a system of N interacting bosons in the Gross-Pitaevskii limit, where N tends to infinity and the scattering length a of the pair potential tends to zero so that Na remains constant. In this limit we prove that the macroscopic dynamics of the system is correctly described by the time-dependent Gross-Pitaevskii equation.

3.4.6 Energy Transport in One-Dimensional Chains: Predictions from the Phonon Kinetic Equation

Herbert Spohn
TU Muenchen
spohn@ma.tum.de

For low density gases in one space-dimension the Boltzmann collision term vanishes. In contrast, for the phonon Boltzmann equation the wave number space is a one-dimensional torus and the kinetic energy is a periodic function. This allows for non degenerate phonon collisions. We investigate the spectrum of the linearized collision operator. For an on-site potential this operator has a spectral gap implying diffusive energy transport, while for the FPU β chain we prove the non integrable decay as $t^{-3/5}$ for the energy current correlation function. This is joint work with Jani Lukkarinen.

3.5 Exactly Solvable Systems

Organizer F. Smirnov (Paris)

3.5.1 Correlation Functions and Hidden Fermionic Structure of the XYZ Spin Chain

Herman Boos
Universität Wuppertal
boos@physik.uni-wuppertal.de

We discuss our recent results on the correlation functions of the XXZ model. The main our point is the application of the exponential formula and the Q-matrix technique for the correlation functions of the XXZ model with 'disordered field'. We obtain the operator in the exponent as a quadratic form wrt some fermionic operators which satisfy the standard anti-commutation relations. In the case of the XX model which corresponds to free fermions the above operators are connected with usual fermionic operators obtained through the well-known Jordan-Wigner transformation.

3.5.2 Particle Decay in Ising Field Theory with Magnetic Field

Gesualdo Delfino
SISSA, Trieste
delfino@fm.sissa.it

The scaling region of the two-dimensional Ising model in a magnetic field is described by a quantum field theory which admits exactly solvable directions and, away from these, displays confinement and unstable particles. We use form factor perturbation theory to determine decay widths for small deviations from critical temperature at non-zero magnetic field.

3.5.3 ABCD—Integrable Models and Ordinary Differential Equations

Roberto Tateo
Torino Univ.
tateo@to.infn.it

We outline a relationship between conformal field theories and spectral problems of ordinary differential equations, and discuss its generalization to models related to A, B, C, D Lie algebras.

3.6 General Relativity

Organizers P. Chrusciel (Tours), H. Nicolai (Golm)

3.6.1 Einstein Spaces as Attractors for the Einstein Flow

Lars Andersson
Albert Einstein Institut, Golm
laan@aei.mpg.de

I will discuss a proof of nonlinear stability of Lorentz cones over Riemannian negative Einstein spaces M of arbitrary dimension, generalizing earlier work in the $3 + 1$ dimensional case. In the higher dimensional case several new phenomena arise. The asymptotic rate of decay depends on the spectral properties of the background geometry. Further, there may be a nontrivial deformation space of negative Einstein spaces on M, examples are provided by Kähler-Einstein spaces. In spacetime dimensions greater than 10, our work allows one to construct large families of vacuum spacetimes with quiescent singularity and asymptotically Friedman behavior in the expanding direction. This talk is based on joint work with Vince Moncrief.

3.6.2 Loop Quantum Cosmology

Martin Bojowald
Penn State Univ.
bojowald@gravity.psu.edu

Focussing on mathematical aspects, this talk will give a review of loop quantum cosmology, which is an application of background independent quantization techniques to cosmological models. Due to discrete spatial geometry as a consequence of the quantization, dynamical equations in such models are difference rather than differential equations. Suitable solutions display typical features in quantum regimes, where they can resolve classical space-time singularities, but should also approach semiclassical behavior in classical regimes. Such solutions can be found using generating function or continued fraction techniques. Semiclassical behavior and corrections to the classical one are derived using effective equations which approximate partial difference equations by ordinary differential equations.

3.6.3 The Red-Shift Effect and Radiation Decay on Black Hole Space-Times

Mihaelis Dafermos
Cambridge
M.Dafermos@dpmms.cam.ac.uk

I will present proofs of uniform decay rates for solutions to the wave equation on various black hole exterior backgrounds. This is joint work with I. Rodnianski.

3.6.4 Angular Momentum-Mass Inequality for Axisymmetric Black Holes

Sergio Dain
Univ. de Cordoba
dain@famaf.unc.edu.ar

In this talk I will discuss the physical relevance of the inequality $\sqrt{J} \leq m$, where m and J are the total mass and angular momentum, for axially symmetric (non-stationary) black holes. In particular, I will prove that for vacuum, maximal, complete, asymptotically flat, axisymmetric initial data, this inequality is satisfied. The proof consists in showing that extreme Kerr is a global minimum of the mass.

3.6.5 Black Hole Entropy in Supergravity and String Theory

Gabriel Cardoso
Universität München
gcardoso@theorie.physik.uni-muenchen.de

We review recent results on subleading corrections to the entropy of extremal black holes in supergravity and string theory.

3.6.6 Infinite-Dimensional R-Symmetry in Supergravity

Axel Kleinschmidt
Universtät Oldenburg
axel.kleinschmidt@aei.mpg.de

Recent work devoted to the study of symmetry structures of supergravity, or the unifying M-theory, has revealed interesting links to the theory of Kac-Moody algebras and their subalgebras. After reviewing these links for the bosonic fields of the theory I will discuss how the fermionic fields fit into the picture. This requires non-trivial results on the mathematical structure of some infinite-dimensional algebras which go beyond the Kac-Moody class. These results permit one to find a common origin of all fermionic fields appearing in the various maximal supergravity theories.

3.7 Operator Algebras

Organizer R. Longo (Rome)

3.7.1 From Vertex Algebras to Local Nets of von Neuman Algebras

Sebastiano Carpi
Università di Chieti e Pescara
carpi@gotham.sci.unich.it

We explain recent results on the connection between vertex algebras and local nets of von Neumann algebras.

(Joint work with Y. Kawahigashi, R. Longo and M. Weiner)

3.7.2 Non-Commutative Manifolds and Quantum Groups

Giovanni Landi
Università di Trieste
landi@units.it

For quite sometime, it has been problematic to endow spaces coming from quantum groups with a noncommutative spin structure and such a possibility has eluded several approaches. We explicitly construct equivariant spectral triples on a variety of examples that include the manifold of quantum SU(2), families of quantum two-spheres, as well as higher dimensional quantum spheres.

3.7.3 L^2 Invariants, Free Probability and Operator Algebras

Dimitri Shlyakhtenko
UCLA
shlyakht@math.ucla.edu

The Cheeger-Gromov L^2 Betti numbers of a discrete group are numerical invariants, going back to Atiyah's work on the equivariant Atiyah-Singer index theorem. On the other hand, Voiculescu has introduced another discrete group invariant, coming from his free probability theory, called the free entropy dimension. Very roughly, this number measures the "asymptotic dimensions" of the sets of approximate embeddings of a group into unitary matrices. We describe our joint work with A. Connes and I. Mineyev that has provided a connection between these numbers.

3.8 Partial Differential Equations

Organizers S. Mueller (Leipzig), I.M. Sigal (Toronto)

3.8.1 Weak Turbulence for Periodic NSL

James Colliander
Univ. of Toronto
colliand@math.toronto.edu

I will describe recent work with G. Staffilani, M. Keel, H. Takaoka and T. Tao. We construct a global-in-time solution of periodic cubic NLS on the 2-torus which transfers the conserved L^2 mass from low frequencies to arbitrarily high frequencies. In particularly, norms measuring smoothness of the solution can grow from their initial size to arbitrarily large size in a finite time. The solution is built using a combinatorial construction on resonant frequencies and the existence of a travelling wave solution in a system of ordinary differential equations which moves from low to high frequencies.

3.8.2 Ginzburg-Landau Dynamics

Stephen Gustafson
University of British Columbia
gustaf@math.ubc.ca

Ginbzburg-Landau type equations have attracted a great deal of interest from mathematicians in recent years. This is a family of nonlinear partial differential equations which describe statics and dynamics in superconductors and superfluids, and which admit interesting localized solutions such as vortices. I will describe some of the recent results on Ginzburg-Landau dynamics.

3.8.3 On the Derivation of Furier's Law

Antti Kupiainen
Helsinki Univ.
ajkupiai@mappi.helsinki.fi

We study the Hamiltonian system made of weakly coupled anharmonic oscillators arranged on a three dimensional lattice and subjected to a stochastic forcing on the boundary. We introduce a truncation of the Hopf equations describing the stationary state of the system which leads to a nonlinear generalized Boltzman equation for the two-point stationary correlation functions. We prove that these equations have a unique solution which, for N large, is approximately a local equilibrium state

satisfying Fourier law that relates the heat current to a local temperature gradient. The temperature exhibits a nonlinear profile. We discuss also implications for the study of Boltzman equations.

3.8.4 TBA

Stefan Mueller
Max Planck Institute for Mathematics in the Sciences, Leipzig
sm@mis.mpg.de

3.8.5 A Criterion for the Logarithmic Sobolev Inequality

Felix Otto
Univ. Bonn
otto@iam.uni-bonn.de

This is joint work with Maria Reznikoff. We present a criterion for the logarithmic Sobolev inequality (LSI) on the product space $X_1 \times \cdots \times X_N$. We have in mind an N-site lattice, unbounded continuous spin variables, and Glauber dynamics. The interactions are described by the Hamiltonian H of the Gibbs measure. The criterion for LSI is formulated in terms of the LSI constants of the single-site conditional measures and the size of the off-diagonal entries of the Hessian of H. It is optimal for Gaussians with positive covariance matrix.

3.8.6 Singular Behaviour in Chemotaxis Models

Juan J. L. Velazquez
Universidad Complutense
JJ_Velazquez@mat.ucm.es

In this talk I will describe some of the singular behaviours that arise in the partial differential equations that describe the phenomenon of chemotactic aggregation. In particular I will describe solutions that generate Dirac masses in finite time. The continuation beyond the blow-up will be also considered as well as the study of the long time asymptotics for some models of chemotactic aggregation where the interaction takes place by means of nondiffusive chemicals.

3.9 Probability Theory

Organizer F. Martinelli (Rome)

3.9.1 Aging in the Infinite Volume REM-Like Trap Model at Low Temperature

Luiz Renato Fontes
IME-USP
lrenato@ime.usp.br

We exhibit the scaling limit of the REM-like trap model at low temperature (with time scaled as the deepest traps) and show that this dynamics exhibits aging (in the proper macroscopic time limit). We also discuss extensions to infinite volume GREM-like trap models at low temperature.

3.9.2 From Planar Gaussian Zeros to Gravitational Allocation

Yuval Peres
UC Berkeley and Microsoft Research
peres@stat.Berkeley.edu

The zeros of the power series with IID complex Gaussian coefficients form a determinantal (Fermionic) process, invariant under hyperbolic isometries. This allows for exact calculation of "hole" probabilities. Recently another Gaussian power series, with Euclidean symmetry, has been investigated in depth. Results of Sodin-Tsirelson reveal a surprising analogy with a four-dimensional Poisson process. We show how the analysis of gravitational allocation for the Euclidean planar Gaussian analytic function (Nazarov-Sodin-Volberg) has led to an analysis of gravitational allocation for the Poisson process in dimensions 3 and higher; each Poisson point is allotted a unit of volume in a translation invariant way, and the diameters of the allocated regions have exponental tails. The argument starts with the classical calculation by Chandrasekar of the total force acting on a point, which has a stable law. (Joint works with S. Chatterjee, R. Peled, D. Romik, B. Virag).

3.9.3 Random Walks in Random Environments in the Perturbative Regime

Ofer Zeitouni
Univ. of Minnesota
zeitouni@math.umn.edu

I will describe recent results and technique used in analysing random walks (and diffusions) in random environment in the perturbative regime, when the environment satisfies certain isotropy conditions.

3.10 Quantum Mechanics

Organizers A. Laptev (Stokholm), B. Simon (Pasadena)

3.10.1 Recent Progress in the Spectral Theory of Quasi-Periodic Operators

David Damanik
CALTECH
damanik@caltech.edu

I will describe recent results and technique used in analysing random walks (and diffusions) in random environment in the perturbative regime, when the environment satisfies certain isotropy conditions.

3.10.2 Recent Results on Localization for Random Schrödinger Operators

Francois Germinet
Universitéé de Cergy-Pontoise
germinet@math.u-cergy.fr

Since Fröhlich and Spencer in 1983, localization of random Schrödinger operators can be studied with a so called multiscale analysis. We shall review some recent developments of this technique and of the kind of localization it implies. It will include the Anderson Bernoulli model as well as the Schrödinger operator with Poisson random potential.

3.10.3 Quantum Dynamics and Enhanced Diffusion for Passive Scalar

Alexander Kiselev
University of Wisconsin
kiselev@math.wisc.edu

Consider a dissipative evolution equation $\psi_t = iL\psi - \epsilon\Gamma\psi$, where Γ, L are self-adjoint operators, $\Gamma > 0$, ϵ small. Can the presence of unitary evolution corresponding to L significantly speed up dissipation due to Γ? The question has a long history in the particular case of the elliptic operators, and has been studied using probabilistic and PDE tools. We prove a sharp result describing the operators L that have this property in the general setting. The methods employ ideas from quantum dynamics. Applications include the classical passive scalar equation and reaction-diffusion equations.

3.10.4 Lieb-Thirring Inequalities, Recent Results

Ari Laptev
KTH, Stockholm
laptev@math.kth.se

Some new recent results concerning Lieb-Thirring inequalities will be discussed. In particular, inequalities are derived for power sums of the real-part and modulus of the eigenvalues of a Schrödinger operator with a complex-valued potential. This is my recent joint paper with Rupert Frank, Elliott Lieb and Robert Seiringer.

3.10.5 Exponential Decay Laws in Perturbation Theory of Threshold and Embedded Eigenvalues

Gheorghe Nenciu
Univ. of Bucharest
Gheorghe.Nenciu@imar.ro

Exponential decay laws for the metastable states resulting from perturbation of unstable eigenvalues are discussed. Eigenvalues embedded in the continuum as well as threshold eigenvalues are considered. Stationary methods are used, i.e. the evolution group is written in terms of the resolvent via Stone's formula and Schur-Feschbach partition technique is used to localize the essential terms. No analytic continuation of the resolvent is required. The main result is about threshold case: for Schrödinger operators in odd dimensions the leading term of the decay rate in the perturbation strength, ε, is of order $\varepsilon^{\nu/2}$ where ν is an odd integer, $\nu \geq 3$.

This is joint work with Arne Jensen.

3.10.6 Homogenization of Periodic Operators of Mathematical Physics as a Spectral Threshold Effect

Tatiana A. Suslina
St. Petersburg State University
suslina@list.ru

In $L_2(\mathbb{R}^d)$, we consider matrix periodic elliptic second order differential operators A admitting a factorization of the form $A = X^*X$. Here X is a homogeneous first order differential operator. Many operators of mathematical physics have such structure. We study a homogenization problem in the small period limit. Namely, for the operator A_ϵ with rapidly oscillating coefficients (depending on x/ϵ), we study the behavior of the resolvent $(A_\epsilon + I)^{-1}$ as ϵ tends to zero. We find approximation for this resolvent in the $(L_2 \to L_2)$-operator norm in terms of the resolvent of the effective operator. For the norm of the difference of the resolvents, we obtain the sharp-order estimate (by $C\epsilon$). The constant in this estimate is controlled explicitly.

Taking the "corrector" into account, we obtain more accurate approximation for the resolvent in the $(L_2 \to L_2)$-operator norm with the error estimate by $C\epsilon^2$. Besides, we find approximation with corrector for the resolvent in the $(L_2 \to H^1)$-operator norm with the error estimate of order $O(\epsilon)$. The obtained results are of new type in the homogenization theory.

The method is based on the abstract operator theory approach for selfadjoint operator families $A(t)$ admitting a factorization of the form $A(t) = X(t)^* X(t)$, $X(t) = X_0 + tX_1$. It turns out that the homogenization procedure for the operator A_ϵ is determined by the spectral characteristics of the periodic operator A near the bottom of the spectrum. Therefore, homogenization procedure can be treated as a threshold effect.

General results are applied to specific operators of mathematical physics: the acoustics operator, the operator of elasticity theory, the Maxwell operator. A special attention is paid to the operators of quantum mechanics, namely, to the Schrödinger operator, the magnetic Schrödinger operator (with sufficiently small magnetic potential), the two dimensional Pauli operator. The effective characteristics for these operators are studied. The effective matrix arising in the homogenization theory is closely related to the tensor of effective masses which is well known in quantum mechanics. It turns out that for the two dimensional periodic Pauli operator the tensor of effective masses is scalar, which attests some hidden symmetry.

The results were obtained in 2001–2006 jointly with M. Sh. Birman.

3.11 Quantum Field Theory

Organizer K. Fredenhagen (Hamburg)

3.11.1 Algebraic Aspects of Perturbative and Non-Perturbative QFT

Christoph Bergbauer
IHES
bergbau@ihes.fr

We review the Connes-Kreimer approach to perturbative renormalization in terms of Hopf and Lie algebras of Feynman graphs which capture the combinatorial aspects of the renormalization procedure. The solution of the Bogoliubov recursion is essentially given by the antipode map of the Hopf algebra of graphs. Important properties can be traced back to 1-cocycles in the Hochschild cohomology of these Hopf algebras. At the same time these 1-cocycles provide the building blocks of Dyson-Schwinger equations and thus a link to non-perturbative results. We finally discuss new ideas on the structure and towards actual solutions of these Dyson-Schwinger equations.

3.11.2 Quantum Field Theory in Curved Space-Time

Stefan Hollands
University of Goettingen
hollands@theorie.physik.uni-goettingen.de

The theory of quantum fields on a curved background is interesting both physically —describing effects such as the creation of primordial fluctuations, particle creation in the expansing universe, black-hole radiance—as well as mathematically, because it combines in an interesting way ideas from differential geometry, analysis, and quantum field theory.

I review recent developments in the field, emphasizing the role and construction the operator product expansion in curved spacetime. In particular, I will argue that properties such as associativity, general covariance, renormalization group flow/scaling, and spectral properties of the quantum field theory are encoded in the operator product expansion. I indicate how this tool may be used to analyze quantitatively dynamical processes in the Early Universe.

3.11.3 String-Localized Quantum Fields, Modular Localization, and Gauge Theories

Jens Mund
Universidade Federal de Juiz de Fora
mund@fisica.ufjf.br

The concept of modular localization introduced by Brunetti, Guido and Longo, and Schroer, can be used to construct quantum fields. It combines Wigner's particle concept with the Tomita-Takesaki modular theory of operator algebras. I shall report on the construction of free fields which are localized in semi-infinite strings extending to spacelike infinity (joint work with B. Schroer and J. Yngvason). Particular applications are: The first local (in the above sense) construction of fields for Wigner's massless "infinite spin" particles; Anyons in $d = 2 + 1$; String-localized vector/tensor potentials for Photons and Gravitons, respectively. Some ideas will be presented concerning the perturbative construction of gauge theories (and quantum gravity) completely within a Hilbert space, trading gauge dependence with dependence on the direction of the localization string.

3.11.4 Quantization of the Teichmüller Spaces: Quantum Field Theoretical Applications

Joerg Teschner
DESY
teschner@mail.desy.de

We will review the geometric interpretation of quantum Liouville theory as a quantum theory of spaces of Riemann surfaces. This interpretation can be used to establish the consistency of the bootstrap construction of Liouville theory in the presence of conformal boundary conditions. It also paves the way towards the study of Liouville theory on higher genus Riemann surfaces. If time permits we will outline a possible extension of this framework to more general conformal field theories.

3.12 2D Quantum Field Theory

Organizer J. Cardy (Oxford)

3.12.1 Lattice Supersymmetry From the Ground Up

Paul Fendley
University of Virginia
fendley@rockpile.phys.virginia.edu

I discuss several models of itinerant fermions which exhibit explicit supersymmetry on the lattice. In $1+1$ dimensions, one model gives a lattice regularization of the Thirring model, and shows how the combinatorial results of Stroganov et al. can be related to supersymmetry. In both $1+1$ and $2+1$ dimensions, we can find models with extensive ground-state entropy. Finally, I present results on a generalized Yangian-like symmetry algebra underlying some of these models.

3.12.2 Analytical Solution for the Effective Charging Energy of the Single Electron Box

Sergei Lukyanov
Rutgers University
sergei@physics.rutgers.edu

A single electron box is a low-capacitance metallic island, connected to an outside lead by a tunnel junction. Over the last decade, correct analytical expressions describing the single electron box in the limit of large tunneling conductance have been the subject of controversial debate. In this talk, we will discuss recent exact

results on the universal scaling behavior of the single electron box in the strong tunneling limit.

3.12.3 Breaking Integrability

Giuseppe Mussardo
SISSA, Trieste
mussardo@he.sissa.it

Thanks to integrable quantum field theories, there has been in recent year new understanding on a large number of models of interest in statistical mechanics or in condensed matter physics, e.g. Ising model in a magnetic field or Sine-Gordon model. Integrability has permitted to determine, for instance, the exact spectrum of many systems, the explicit determination of the correlation functions of their order parameters, as well as their thermodynamical properties. In the seminar there will be discussed two methods which permits to extend this analysis also to non-integrable models: the first one is based on the Form Factor Perturbation Theory while the second is based on semi-classical techniques. Both approaches will be then illustrated by studying in details the non-integrable features of theories with kink excitations, like for instance the Ising model or Double Sine Gordon. We present the evolution of the spectrum of the stable particles and the computation of the decay width of the unstable ones.

3.13 Quantum Information

Organizers A. Holevo (Moscow), M. B. Ruskai (Medford)

3.13.1 One-and-a-Half Quantum de Finetti Theorems

Matthias Christandl
Cambridge
mc380@cam.ac.uk

When n-k systems of an n-party permutation invariant density matrix are traced out, the resulting state can be approximated by a convex combination of tensor product states. This is the quantum de Finetti theorem. Here we show that an upper bound on the trace distance of this approximation is given by $2kd^2/n$, where d is the dimension of the system, thereby improving previously known bounds. Our result follows from a more general approximation theorem for states in representations of the unitary group by coherent states.

For the class of symmetric Werner states, which are invariant under both the permutation and unitary groups, we give a second de Finetti-style theorem (our "half" the-

orem). It arises from a combinatorial formula for the distance of symmetric Werner states to product Werner states, making a connection to the recently defined shifted Schur functions. This formula also provides us with useful examples that allow us to conclude that finite quantum de Finetti theorems (unlike their classical counterparts) must depend on the dimension d. This is joint work with Robert Koenig, Graeme Mitchison and Renato Renner.

3.13.2 Catalytic Quantum Error Correction

Igor Devetak
University of Southern California
devetak@usc.edu

We exhibit a natural generalization of the stabilizer formalism for entanglement-assisted quantum error correction. Conventional stabilizer codes for quantum channels without entanglement assistance are equivalent to isotropic (or self-orthogonal T) symplectic codes. When entanglement assistance is included, the isotropicity condition is no longer necessary. A catalytic quantum code is one which borrows the use of a perfect quantum channel and returns it at the end of the protocol. One of the consequences of the above result is that any classical code over GF(4) can be made into a catalytic quantum code. In particular, classical codes over GF(4) attaining the Shannon limit correspond to catalytic quantum codes attaining the hashing bound.

3.13.3 Quantum State Transformations and the Schubert Calculus

Patrick Hayden
McGill University
patrick@cs.mcgill.ca

The problem of relating the eigenvalues of a density operator to those of its reductions, known as the quantum marginal problem, is closely connected to determining the amount of communication required to convert one entangled quantum state into another. I'll develop this connection and show how the solution to a restricted version of the marginal problem can be used to extract simple conditions governing the existence of transformations in particular cases.

3.13.4 The Local Hamiltonian Problem

Julia Kempe
CNRS & University of Paris
kempe@lri.fr

Most physical systems are described by a sum of local Hamiltonians, i.e. Hamiltonians that act on a few particles each. Computing the ground state energy of these

systems is notoriously hard in general and has been studied in many settings, most importantly on square lattices. Kitaev was the first to cast the problem in complexity theoretic terms; he showed that the 5-Local Hamiltonian problem is as hard as any problem in QMA, the quantum analogue of NP. We will review the status of the problem since then with some new rigorous perturbation theory techniques on the way and also give a connection to adiabatic quantum computing.

3.13.5 The Information-Disturbance Tradeoff and the Continuity of Stinespring's Representation

Dennis Kretschmann
TU Braunschweig
d.kretschmann@tu-bs.de

Stinespring's famous dilation theorem is the basic structure theorem for quantum channels: it states that every quantum channel (i.e., completely positive and trace preserving map) arises from a unitary evolution on a larger system. The theorem not only provides a neat characterization of the set of permissible quantum operations, but is also a most useful tool in quantum information science.

Here I will present a continuity theorem for Stinespring's dilation: if two quantum channels are close in cb-norm, then we can always find unitary implementations which are close in operator norm, with dimension-independent bounds. This result can be seen as a generalization of Uhlmann's theorem from states to channels and allows to derive a formulation of the information-disturbance tradeoff in terms of quantum channels, as well as a continuity estimate for the no-broadcasting theorem. Other applications include a strengthened proof of the no-go theorem for quantum bit commitment.

Joint work with D. Schlingemann and R. F. Werner.

3.13.6 Locality Estimates for Quantum Spin Systems

Robert Sims
University of Vienna
robert.sims@univie.ac.at

We review some recent results that express or rely on the locality properties of the dynamics of quantum spin systems. In particular, we present a slightly sharper version of the recently obtained Lieb-Robinson bound on the group velocity for such systems on a large class of metric graphs. Using this bound we provide expressions of the quasi-locality of the dynamics in various forms, present a proof of the Exponential Clustering Theorem, and discuss a multi-dimensional Lieb-Schultz-Mattis Theorem.

3.14 Random Matrices

Organizers J. Baik (Ann Arbor), J. Harnad (Montréal)

3.14.1 Exact Solution of the Six-Vertex Model with Domain Wall Boundary Conditions

Pavel M. Bleher
Indiana University Purdue University Indianapolis
bleher@math.iupui.edu

The six-vertex model, or the square ice model, with domain wall boundary conditions (DWBC) has been introduced and solved for finite N by Korepin and Izergin. The solution is based on the Yang-Baxter equations and it represents the free energy in terms of an $N \times N$ Hankel determinant. Paul Zinn-Justin observed that the Izergin-Korepin formula can be re-expresses in terms of the partition function of a random matrix model with non-polynomial interaction. We use this observation to obtain the large N asymptotic of the six-vertex model with DWBC in the disordered phase. The solution is based on the Riemann-Hilbert approach and the Deift-Zhou nonlinear steepest descent method. As was noticed by Kuperberg, the problem of enumeration of alternating sign matrices (the ASM problem) is a special case of the six-vertex model. We compare the obtained exactsolution of the six-vertex model with known exact results for the 1, 2, and 3 enumerations of ASMs, and also with the exact solution on the so-called free fermion line. We prove the conjecture of Zinn-Justin that the partition function of the sic-vertex model with DWBC has the asymptotics, $Z_N \sim CN^{\kappa}e^{N^2 f}$ as $N \to \infty$, and we find the exact value of the exponent κ.

3.14.2 Probabilities of a Large Gap in the Scaled Spectrum of Random Matrices

Igor Krasovsky
Brunel Univ.
mastiik2@brunel.ac.uk

In the Gaussian Unitary Ensemble of random matrices, the probability of an interval (gap) without eigenvalues in the spectrum (rescaled in a standard way) is given by the sine-kernel Fredholm determinant in the bulk of the spectrum, and by the Airy-kernel Fredholm determinant at the edge. We calculate asymptotics of these determinants for a large gap proving the conjectures of Dyson, Tracy and Widom about the multiplicative constant in these asymptotics. Our method uses analysis of a Riemann-Hilbert problem and can be adapted to calculate such constants in asymptotics of a number of similar determinantal correlation functions of random

matrix theory and exactly solvable models. The talk is based mostly on joint works with P. Deift, A. Its, and X. Zhou.

3.14.3 Random Matrices, Asymptotic Analysis, and d-bar Problems

Kenneth McLaughlin
University of Arizona
mcl@math.arizona.edu

The aim of the research is to study random matrix models for which the external field is outside the analytic class.

3.14.4 Central Limit Theorems for Non-intersecting Random Walks

Toufic Suidan
UC Santa Cruz
tsuidan@ucsc.edu

We describe several central limit theorems for non-intersecting random walks. The limiting distributions which arise are related to classical random matrix theory. Connections to last passage percolation and other models will be discussed. This work is joint with Jinho Baik.

3.14.5 On the Distribution of Largest Eigenvalues in Random Matrix Ensembles

Alexander Soshnikov
UC Davis
soshniko@math.ucdavis.edu

In the talk, we will consider the Wigner and Wishart ensembles of random matrices and their generalizations. We will discuss the spectral properties of random matrices from these ensembles, in particular the distribution of the largest (smallest) eigenvalues.

3.14.6 Non-Intersecting Brownian Excursions

Craig A. Tracy
UC Davis
tracy@math.ucdavis.edu

A Brownian excursion is a Brownian path starting at the origin at time $t = 0$ and ending at the origin at time $t = 1$ and conditioned to remain positive for $0 < t < 1$.

We consider n such Brownian excursion paths conditioned to be nonintersecting. Using techniques from random matrix theory, we discuss this process. This is joint work with H. Widom.

3.15 Stochastic PDE

Organizer W.E. (Princeton)

3.15.1 Degenerately Forced Fluid Equations: Ergodicity and Solvable Models

Jonathan C. Mattingly
Duke University
jonmmath.duke.edu

I will present some recent results on the existence of spectral gaps for the 2D Navier Stokes equation under very degenerate stochastic forcing. I will use these results to show that the statistical steady states depend in a nice fashion on the parameters of the problem.

I will close with some interesting results on some exactly solvable models of energy transport in stochastic systems.

3.15.2 Microscopic Stochastic Models for the Study of Thermal Conductivity

Stefano Olla
Université de Paris, Dauphine
ollaceremade.dauphine.fr

Anomalous large thermal conductivity has been observed numerically and experimentally in one- and two-dimensional systems. We study the thermal conductivity of an infinite system of oscillators whose Hamiltonian dynamics is perturbed by a multiplicative (non-linear) noise conserving energy and momentum. The decay of the energy current correlation function $C(t)$ can be estimated. In the harmonic case $C(t)$ can be computed explicitly and we prove that thermal conductivity is finite if $d = 3$ or if an on-site potential is present, while it is infinite if $d = 1$ or 2. This result clarifies the role of conservation of momentum and dispersion relation in the anomalous thermal conductivity in low dimensions. We also discuss Fourier's law and evolution of energy fluctuations. This is a joint work with Giada Basile and Cedric Bernardin.

3.15.3 Boundary Effects on the Interface Dynamics for the Stochastic Allen-Cahn Equation

Stella Brassesco
IVIC, Caracas
sbrasses@ivic.ve

We consider a stochastic perturbation of the Allen–Cahn equation in a bounded interval $[-a, b]$ with boundary conditions fixing the different phases at a and b. We investigate the asymptotic behavior of the front separating the two stable phases in the limit $\epsilon \to 0$, when the intensity of the noise is $\sqrt{\epsilon}$ and $a, b \to \infty$ with ϵ. In particular, we prove that it is possible to choose $a = a(\epsilon)$ such that in a suitable time scaling limit, the front evolves according to a one-dimensional diffusion process with a nonlinear drift accounting for a "soft" repulsion from a. We finally show that a "hard" repulsion can be obtained by an extra diffusive scaling.

3.16 String Theory

Organizers N. Berkovits (São Paulo), R. Dijkgraaf (Amsterdam)

3.16.1 Topological Strings and (Almost) Modular Forms

Mina Aganagic
UC Berkeley
minamath.berkeley.edu

The mapping class group Γ is a symmetry of the topological string theory on a Calabi-Yau. This symmetry has a natural realization in the quantum theory, and constrains the topological string partition function. The topological string amplitudes are either holomorphic, quasi-modular forms of Γ, or modular forms which are almost holomorphic. Moreover, at each genus, certain combinations of the amplitudes have to be both holomorphic and modular invariant.

3.16.2 Gauge Theory and Link Homologies

Sergei Gukov
Harvard
gukovsakharov.physics.harvard.edu

The main goal of this talk is to explain the physical interpretation of the existing link homologies—such as the Khovanov homology or knot Floer homology—and to propose their various generalizations motivated from physics. In particular, starting with a brief introduction into knot homology theories, I will describe a frame-

work for unifying the sl(N) Khovanov-Rozansky homology (for all N) with the knot Floer homology. This unification, based on the interpretation in topological string theory, is accomplished by a new triply graded homology theory which categorifies the HOMFLY polynomial. Further insights can be obtained by realizing knot homologies in gauge theory. As I will explain in the main part of the talk, surface operators in gauge theory and braid group actions on categories play an important role in such realizations.

3.16.3 Non-Geometric String Backgrounds

Chris Hull
Imperial College
c.hullimperial.ac.uk

In string theory, the standard field theory symmetries of diffeomorphisms and gauge symmetries are augmented by stringy duality symmetries that have no field theory analogue. Conventional spacetime manifolds are constructed from local patches equipped with a metric and gauge and matter fields, and these are glued together using diffeomorphisms and gauge symmetries. In string theory there is the possibility of also using duality symmetries to glue together local spacetime patches, resulting in a "non-geometric background" that has no conventional geometric description. This suggests that in string theory the conventional geometric spacetime picture should be replaced by something more general, allowing a much wider class of string theory backgrounds than has hitherto been considered. The purpose of this talk is to explore such non-geometric backgrounds and some of their implications.

3.16.4 Topological Reduction of Supersymmetric Gauge Theories and S-Duality

Anton Kapustin
Caltech
kapustintheory.caltech.edu

I discuss topological and semi-topological reduction of $N = 4$ and $N = 2$ field theories on a Riemann surface. In the $N = 4$ case, this relates S-duality of $4d$ gauge theories with mirror symmetry of the Hitchin moduli space. In the $N = 2$ case, the reduction yields a half-twisted sigma-model with Hitchin moduli space as a target.

3.16.5 Phase Transitions in Topological String Theory

Marcos Marino Beiras
CERN
Marcos.Marino.Beirascern.ch

Topological strings in Calabi–Yau manifolds undergo phase transitions at small distances that signal the onset of quantum geometry. In this talk, after a brief review, I analyze this phenomenon when the Calabi–Yau is a bundle over a sphere. Mathematically, this theory can be regarded as a deformation of Hurwitz theory. The resulting models exhibit critical behavior, but the universality class of the transition corresponds to pure 2d gravity, and one can define a double–scaled theory at the critical point which is governed by the Painleve I equation. It is also possible to induce multicritical behavior. I will also comment on the implications of this result for the conjectural nonperturbative completion of these models.

3.16.6 Hyper-Multiplet Couplings in $N = 2$ Effective Action

Pierre Vanhove
CEA Saclay
pierre.vanhovecea.fr

We will address the analysis of the quantum corrections to the hypermultiplet geometry of $N = 2$ supergravity, with some emphasis on the case of the of universal (dilaton) hypermutiplet. We will discuss some special contributions to the $N = 2$ effective action in the hypermultiplet sector from higher-genus string theory amplitude computation.

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