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Exact Results in Model Statistical Systems

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Final Report for Period: 07/2006 - 06/2007 Principal Investigator: Kleban, Peter H. Organization: University of Maine Submitted By:

Title:

Exact Results in Model Statistical Systems

Project Participants

Senior Personnel

Name: Kleban, Peter Worked for more than 160 Hours: Yes Contribution to Project: Peter Kleban is the PI for this project.

Post-doc

Graduate Student

Name: Fiala, Jan

Worked for more than 160 Hours: Yes

Contribution to Project:

This grant has given considerable help to the education of Jan Fiala, who has been awardede a PhD. in Physics. JanÆs thesis involves a study of the thermodynamics of the Farey fraction spin chain. The research assistantship provided by this grant has greatly aided his progress. Jan has several publications, has attended a workshop and several meetings, and given two talks (one invited) on his research. In addition, he has learned several new techniques, e.g. renormalization group. He currently holds a postdoctoral position at Clark University.

Name: Simmons, Jacob

Worked for more than 160 Hours: Yes

Contribution to Project:

Jacob has completed his PhD in Physics. His research involves applying conformal field theory to percolation in two dimensions. His thesis was very successful, resulting in four publications to date, with two more almost completed. The most important result of his thesis solves an outstanding problem in percolation using a novel method that promises to shed light on some underlying, not yet understood symmetry. He attended several meetings and gave two talks. He has begun a postdoctoral position with J. Cardy at Oxford.

Undergraduate Student

Name: Tkachuk, Vitaly

Worked for more than 160 Hours: Yes

Contribution to Project:

Vitaly started as a freshman in September 2002 as an Electrical and Computer Engineering major. Despite a very heavy course load, he has written a C++ program to enumerate the Farey spin chain partition function (this may be extended to calculate other statistical quantities). This led him into some interesting computational areas, i.e. how to write the program without ôifö statements, and how to do the computation via parallel processing. He has also interacted extensively with my graduate student Jan Fiala.

Technician, Programmer

Other Participant

Submitted on: 07/05/2007 **Award ID:** 0203589

Organizational Partners

Max Planck Institute for Mathematics

Collaboration with Prof. Don Zagier, who is at this Institute most of the year.

College de France

Collaboration with Prof. Don Zagier, who is there during the fall.

University of Nottingham

The PI is collaborating with Prof. N. Diamantis, a number theorist at the University of Nottingham. Nikos is an expert on higher-order modular forms, modular objects that arise from the paper by the PI and Don Zagier. The object of our collaboration is to apply results in this area to percolation (or SLEs).

Queen Mary, University of London

The PI is collaborating with Prof. Thomas Prellberg, who is in the dynamical systems group at Queen Mary, University of London. We are applying ideas and techniques from dynamical systems to the Farey spin chain model.

University of Michigan Ann Arbor

We have been collaborating with Prof. R. M. Ziff, Department of Chemical Engineering (and Michigan Center for Theoretical Physics). Bob is a recognized expert in computer simulations of percolation. We have one publication in Phys. Rev. Letters, and several others supported by renewal award no. DMR-0536927.

Cardiff University

The PI is collaborating with Prof. A. Zhigliavsky, School of Mathematics, on proving a new result involving Farey fractions. He has provided some travel support.

Other Collaborators or Contacts

Collaborations:

1) Don Zagier, Max-Planck-Insitut f³r Mathematik, Bonn (and CollÞge de France, Paris). We co-authored a paper on crossing probabilities.

2) Ali Ízl³k, Mathematics Department, University of Maine. He is a long-time collaborator. He co-authored a paper on the Farey spin chain (together with the PI and Jan Fiala).

3) Nikolaos Diamantis, Mathematics, University of Nottingham. Nikos is an expert on higher-order modular forms, which arise from the PI's paper with Don Zagier. We are attempting to apply this theory to percolation (or SLEs).

4) Thomas Prellberg, Mathematics, Queen Mary, University of London. Thomas is an expert in dynamical systems. We are collaborating on investigating the Farey spin model using operator theory methods.

5) Robert M. Ziff, Department of Chemical Engineering, University of Michigan. Bob is a recognized expert on simulating percolation. We are collaborating in investigating critical 2-D percolation.

Contacts in the area of crossing probabilities and Stochastic L÷wner Evolution: 2002-2003: The PI had contacts with J. Cardy, T. Spencer and S. Smirnov during several visits to the Institute for Advanced Study. He also had contact with W. Werner during a visit to the Institut Henri PoincarÚ, Paris. 2003-2004: Contacts with W. Werner (Paris and Princeton), R. Friedrich (Princeton). 2004-2005: Contacts with J. Cardy, R. Friedrich, S. Sheffield (Princeton). 2005-2006:

Contacts with M. Aizenman (Princeton) and N. Diamantis, University of Nottingham.

2006-2007:

Contacts with M. Aizenman, J. Cardy (Princeton) and N. Diamantis, University of Nottingham, Don Zagier, CollPge de France.

Contacts in the area of the Farey spin chain: 2003-2004: T. Prellberg, Universitaet Clausthal. 2004-2005: J. Lebowitz, Rutgers University. 2006-2007: T. Prellberg and O. Bandtlow, Queen Mary, University of London, A. Zhigliavsky, Cardiff University, Don Zagier and M-S. Dupertuis, CollÞge de France.

Activities and Findings

Research and Education Activities: (See PDF version submitted by PI at the end of the report)

Findings: (See PDF version submitted by PI at the end of the report)

Training and Development:

This grant has been essential for the education of Jan Fiala, who has completed his PhD in Physics. Jan's thesis involves a study of the thermodynamics of the Farey fraction spin chain. The research assistantship provided by this grant has greatly aided his progress. Jan has co-authored a publication, gone to a workshop and several meetings, and given two talks (one invited) on his research. In addition, he has learned several new techniques, e.g. renormalization group. He finished his degree in December 2004 and has moved on to a postdoctoral position at Clark University.

In addition, an undergraduate, Vitaly Tkachuk, has been involved in this project. Vitaly started as a freshman in September 2002 as an Electrical and Computer Engineering major. Despite a very heavy course load, he has written a C++ program to enumerate the Farey spin chain partition function (this will probably be extended to calculate other statistical quantities). This led him into some interesting computational areas, i.e. how to write the program without 'if' statements, and how to do the computation via parallel processing.

A second graduate student, Jacob J. H. Simmons, has been involved on the project. Jake has completed his PhD. in Physics. His thesis involves applying conformal field theory to percolation in two dimensions. The research assistantship provided by this grant has greatly aided his progress. Jake is co-author on a paper in this area, supported under this grant, and on several others supported under continuation Grant No. DMR-0536927. Jake is currently a postdoctoral fellow with J. Cardy in Oxford.

Outreach Activities:

Journal Publications

Peter Kleban and Don Zagier, "Crossing Probabilities and Modular Forms", Journal of Statistical Physics, p. 431, vol. 113, (2003). Published, 10.1023/A:1026012600583

Jan Fiala, Peter Kleban and Ali Ozluk, "The Phase Transition in Statistical Models Defined on Farey Fraction", Journal of Statistical Physics, p. 73, vol. 110, (2003). Published, 10.1023/A:1021014627403

Jan Fiala and Peter Kleban, "Generalized Number Theoretic Spin Chain-Connections to Dynamical Systems and Expectation Values", J. Stat. Phys., p. 553, vol. 121, (2005). Published, 10.1007/s10955-005-7579-8

Thomas Prellberg, Jan Fiala and Peter Kleban, "Cluster Approximation for the Farey Fraction Spin Chain", J. Stat. Phys., p. 455, vol. 122, (2006). Published,

Peter Kleban, Jacob J. H. Simmons, and Robert M. Ziff, "Anchored Critical Percolation Clusters and 2-D Electrostatics", Phys. Rev. Letters, p. 115702, vol. 97, (2006). Published, 10.1103/PhysRevLett.97.115702

Jan Fiala and Peter Kleban, "Thermodynamics of the Farey Fraction Spin Chain", J. Stat. Phys., p. 1471, vol. 116, (2004). Published, 10.1023/B:JOSS.0000041727.66775.d3

Jan Fiala and Peter Kleban, "Intervals Between Farey Fractions in the Limit of Infinite Level", Acta Arithmetica, p., vol., (2007). Submitted,

Jacob J. H. Simmons, Peter Kleban, and Robert M. Ziff, "Percolation crossing formulas and conformal field theory", J. Phys. A: Math. Theoret. (fast track communication), p., vol., (2007). Accepted,

Jacob J. H. Simmons, Peter Kleban, and Robert M. Ziff, "Exact factorization of correlation functions in 2-D critical percolation", arXiv: 0706.4105, p., vol., (2007). preprint,

Books or Other One-time Publications

Web/Internet Site

URL(s):

http://www.maths.dur.ac.uk/events/Meetings/LMS/2006/DSSM/talks.html

Description:

This URL points to the abstract and WMV and PDF versions of my talk on the Farey fraction spin chain at the London Mathematical Society Durham Symposium on Dynamical Systems and Statistical Mechanics.

Other Specific Products

Contributions

Contributions within Discipline:

The PI's publication with Don Zagier, 'Crossing Probabilities and Modular Forms', J. Stat. Phys. 113, 431-454 (2003) [arXiv:

math-ph/0209023], probably consitutes the most significant advance. This paper considers crossing probabilities, i.e. the probability of finding a path from one side of a region to the other, on (two-dimensional) shapes such as rectangles. It is for systems 'at criticality', e.g. a percolating system at its percolation point, the condition in which an infinite connected cluster exists as the size of the region grows. What we show is a surprising and interesting connection between crossing and modular forms, mathematical functions of great interest to number theorists. The connection is unexpected because shapes like rectangles do not posses the symmetry generally required for modular forms to be applicable. Thus our result suggests some hidden symmetry in these systems. A little more technically, our results are of interest because by using a simple assumption we can completely characterize the crossing probabilities using modular arguments. The results apply to both critical percolation and Stochastic L÷wner Evolution (SLE) processes.

Our second publication is Jan Fiala, Peter Kleban and Ali Ízl³k, 'The Phase Transition in Statistical Models Defined on Farey Fractions', J. Stat. Phys. 110, 73-86 (2003) [arXiv: math-ph/0203048]. This shows rigorously that the phase transition in the Farey fraction spin chain (a model developed by the PI and A. Ízl³k) is of the type called 'second-order'. This generally means that the thermodynamic phases at the transition point become identical, i.e. merge smoothly into each other. In our model we find an explicit mathematical expression for the free energy (it goes as t/ln(t), where t = T-Tc) for temperatures above the phase transition (t > 0). This is interesting, since the magnetization in this model is already known to be completely saturated for t < 0 and jump to 0 at the phase transition, which suggests a first-order transition, i.e. one in which distinctly different phases co-exist at the transition point. Reconciling these facts is one of our current research goals.

In 'Thermodynamics of the Farey Fraction Spin Chain', by J. Fiala and P. Kleban, J. Stat. Phys. 116, pp. 1471-1490 (2004) [arXiv:

math-ph/0310016] we extend previous work on the thermodynamics of this model by introducing an external magnetic field h. From rigorous and renormalization group arguments, we determine the phase diagram and phase transition behavior of the extended model. Our results are fully consistent with scaling theory (for the case when a 'marginal' field is present) despite the unusual nature of the transition for h=0.

Our next paper is 'Generalized Number Theoretic Spin Chain-Connections to Dynamical Systems and Expectation Values', by J. Fiala and P. Kleban, J. Stat. Phys. 121, 553 - 577 (2005) [arXiv: math-ph/0503030]. Here we use an extended definition of the Farey partition function suggested by Don Zagier. It allows us to make a very simple and explicit connection between the partition function and the transfer operator of the associated dynamical system, the Farey map. Such a connection was known previously, but it was less direct and complete. In addition, we are able to evaluate certain correlation functions exactly (as functions of the free energy) in the Farey model. These exhibit some rather unusual behavior, which is associated with the mechanism of the phase transition.

The next paper is 'Cluster Approximation for the Farey Fraction Spin Chain' by Thomas Prellberg, Jan Fiala and Peter Kleban, J. Stat.Phys. 123 455-471 (2006) [arXiv: cond-mat/0507662]. Here we develop a cluster approximation, based on dynamical system ideas, and apply it to the Farey model with an external field. We reproduce the rigorous asymptotic temperature dependance of the free energy near the phase transition at h = 0. The phase diagram is similar to what is found using renormalization group, but some interesting differences appear.

The paper ôIntervals Between Farey Fractions in the Limit of Infinite Levelö, by Jan Fiala and Peter Kleban, submitted to Acta Arithmetica [arXiv: math-ph/0505053] contains an interesting result on the sum of lengths of half of the intervals between ônew' Farey fractions. It proves, rigorously, that the lim inf of this sum vanishes in the limit of infinite level. The numerical evidence makes it clear that the limit of this sum vanishes. This very simple geometric property of the Farey fractions is not very apparent. The intervals chosen are alternating, and there seems no obvious reason why the sum of their lengths should vanish in this limit. Futher work is underway to understand this point. This work was also supported by the continuation grant, and the NSF grant for the Kavli Institute, where part of it was done, while the PI attended a workshop.

In 'Anchored Critical Percolation Clusters and 2-D Electrostatics, by Peter Kleban, Jacob J. H. Simmons, and Robert M. Ziff, Phys. Rev. Letters 97, 115702 (2006) [arXiv: cond-mat/0605120], we consider the densities of clusters, at the percolation point of a two-dimensional system, which are anchored in various ways to an edge. These quantities are calculated by use of conformal field theory and computer simulations. We find that they are given by simple functions of the potentials of 2-D electrostatic dipoles, and that a kind of superposition cum factorization applies. Our results broaden this connection, already known from previous studies, and we present evidence that it is more generally valid. An exact and universal result similar to the Kirkwood superposition approximation emerges.

Some extensions of this work are in the preprint ôExact factorization of correlation functions in 2-D critical percolationö, by Jacob J. H. Simmons, Peter Kleban, and Robert M. Ziff [arXiv: 0706.4105]. We will probably submit this to Phys. Rev. E.

Perhaps the most significant result of Jake SimmonsÆ thesis is about to be published: ôPercolation crossing formulas and conformal field theoryö, by Jacob J. H. Simmons, Peter Kleban, and Robert M. Ziff, J. Phys. A: Math. Theor. (fast track communication), to appear [arXiv: 0705.1933]. I quote the (only) refereeÆs report in full: ôThis interesting paper shows how various percolation crossing formulas can be unified by positing an operator identity in the CFT, of a rather novel form. This not only leads to new formulae, it probably sheds light on possible hidden symmetries in percolation CFT. The paper is well-written and deserves publication.ö

I expect two more papers to appear, on applications of percolation crossing formulas to regions of trapezoidal shapes, and a technical paper on calculating operator product expansion coefficients, some of which are used in the above. Both of these are close to preprint form at present. Both these and the last two papers mentioned are also supported by the continuation grant.

Contributions to Other Disciplines:

The PLÆs experience in conformal field theory (and more pertinently, conformal mapping) led to some useful results in what is seemingly a very different area. The PI is involved (with others) in a project to develop spectrometers with greatly improved throughput. This has been supported by NSF (under the MRI grant DMR-9977800 ôDevelopment of a Fourier transform-based time-of-flight spectrometer with ultra-high resolutionö) and also by a grant from the Maine Technology Institute, which funded the incorporation of a company, Stillwater Scientific Instruments, of which the PI is a founding partner. The instrument involves a Bradbury-Nielsen gate (two interleaved conducting ôcombsö with opposite voltages), which interrupts the beam of ions when voltage is applied to it, thus creating time-of-flight pulses. The PI has derived new analytical formulas for the ion scattering angles (especially those not large enough to cause the ions to miss the detector, so they are erroneously counted) and also for the number of ions with a given excess voltage (ôenergy corruptionö) when the voltage is turned on or off. These quantities are of central importance in understanding the performance of the instrument.

Contributions to Human Resource Development:

This grant has provided an opportunity for Vitaly Tkachuk, and undergraduate Electrical Engineering major, to participate in research.

Contributions to Resources for Research and Education:

Contributions Beyond Science and Engineering:

Conference Proceedings

Categories for which nothing is reported:

Activities and Findings: Any Outreach Activities Any Book Any Product Contributions: To Any Resources for Research and Education Contributions: To Any Beyond Science and Engineering Any Conference The PI and Don Zagier, a very eminent number theorist, have found a surprising and suggestive connection between crossing probabilities on fully-finite regions at criticality (e.g. rectangles at the percolation point) and modular forms, mathematical functions of great interest to number theorists. The connection is unexpected because shapes like rectangles do not posses the symmetry generally required for modular forms to be applicable. Thus our result suggests some hidden symmetry in these systems. It is of interest because by using a simple assumption we can completely characterize the crossing probabilities using modular arguments. The results apply to both critical percolation and Stochastic Löwner Evolution (SLE) processes.(Note that this research was done, in the main, before the grant was awarded, but not completed until after the grant began.)

The PI, his graduate student Jan Fiala, and collaborator Ali Özlük found some new results for the Farey spin chain model. First, we proved rigorously that the phase transition in the Farey fraction spin chain (a model developed by the PI and A. Özlük) is (barely) second-order, with free energy going as $t/\ln(t)$ for temperatures above the phase transition (t > 0). This is interesting. The magnetization in this model is already known to be completely saturated for t < 0 and jump to 0 at the phase transition, which suggests a first-order transition. A second finding proves that the same behavior applies to several other one-dimensional models defined on the Farey fractions.

(Note that this research was done after the NSF proposal was submitted but before it was funded.)

In order to better understand the thermodynamics of the Farey fraction model, we have done considerable work on extending the model by including an external field h. We have been able to prove that the free energy exists when this is done (since the model is defined in an unusual way, this is not completely obvious). In addition, we have shown that the model is saturated for all h at low temperatures (t < 0). The rest of the phase diagram is being evaluated using renormalization group techniques. Despite the apparent "mixed" nature of the phase transition (partly first and partly second-order), it appears that its thermodynamics is fully consistent with scaling theory, if a marginal field is present.

Another project involves an extension of the Farey partition function suggested to us by Don Zagier. This greatly simplifies the connection of the partition function with the Lewis three-term (functional) equation and other work in operator theory, which is in turn connected with the Selberg zeta function, of great current interest to number theorists. This approach has been fruitful in two ways. First, it has allowed us to find a very explicit and simple connection between the Farey partition function and the transfer operator of the Farey map. Secondly, we have been able to evaluate, exactly, certain correlation functions in the Farey system.

Working with Prof. Thomas Prellberg, we have developed a new approach to the Farey fraction spin chain in an external field h. Utilizing ideas from dynamical systems, the free energy of the model is derived by means of an effective cluster energy approximation.

This approximation is valid for divergent cluster sizes, and hence appropriate for the discussion of the magnetizing transition. We calculated the phase boundaries and the scaling of the free energy. At h=0 we reproduce the rigorously known (from our previous work) asymptotic temperature dependence of the free energy. For h different from zero, our results are largely consistent with those found previously using mean field theory and renormalization group arguments.

More recently, by use of operator identities, we have done considerable work on extending this calculation into a completely rigorous derivation of the free energy as a function of *both* the temperature and the magnetic field, in the vicinity of the second-order phase transition point. This research is almost completed; what remains are some technical matters relating to the precise definition of the function spaces required. We do not anticipate any great difficulties here. When completed, this calculation will be one of the only rigorous results of this type.

We have also found an interesting result on the sum of lengths of half of the intervals between "new" Farey fractions. We have proved, rigorously, that the lim inf of this sum vanishes in the limit of infinite level. The numerical evidence makes it clear that the limit of this sum vanishes. This very simple geometric property of the Farey fractions is not very apparent. The intervals chosen are alternating, and there seems no obvious reason why the sum of their lengths should vanish in this limit. Further work on interpreting this property via the Farey map, which is a model of intermittency in chaos is underway in collaboration with Prof. A. Zhigliavsky.

In collaboration with Prof. R. M. Ziff, the PI and his graduate student Jacob Simmons have examined the behavior of clusters attached to boundaries in 2-D critical percolation. In particular, we consider the densities of such clusters. These quantities are calculated by use of conformal field theory and computer simulations. We find that they are given by simple functions of the potentials of 2-D electrostatic dipoles, and that a kind of superposition cum factorization applies. Our results broaden this connection, already known from previous studies, and we present evidence that it is more generally valid. An exact and universal result reminiscent of the Kirkwood superposition approximation emerges.

In addition, several other exact (and universal) factorizations of higher-order correlation functions arise. We are not aware of any other exact result of this type in theory of fluids. Further, it appears that this kind of factorization also applies for correlations on Fortuin–Kastelyn clusters at the critical points of the two–dimensional q–state Potts models. This work is still ongoing, and also supported under our continuation grant.

Perhaps the most significant result of Jake Simmons' thesis posits a novel operator identity in conformal field theory (for c = 0, which applies to percolation). This gives rise to several new crossing formulas, which are used to unify the previously known crossing results. Further, it probably sheds light on hidden symmetries in percolation.

One major goal of our research is a deeper understanding of critical percolation in two dimensions. This is an important and very extensively studied model system, to which we are bringing new and unexpected approaches. We treat this system by means of conformal field theory, number theory and computer simulations. The other main goal is a study of the phase transition of the Farey fraction spin chain, a set of one–dimensional models that exhibits interesting phase transition behavior. These spin chains are connected to multifractals and dynamical systems. We investigate them with various analytical methods, including operator theory and number theory, and to some extent computer simulation.

Our major educational goal is the training of graduate students in these areas of study. To some extent, undergraduates have also been involved in the research. In addition, the talks given at various institutions contribute to the diffusion of knowledge and to training in physics and mathematics, mainly on the graduate level.

Presentations:

<u>2002-2003</u>:

Peter Kleban, invited talk on "Scaling theory for the Farey fraction spin chain", workshop on the Selberg zeta function, Max-Planck-Insitut für Mathematik, Bonn, June 2002.

Jan Fiala, invited talk on "Phase transition in the Farey fraction spin chain", workshop on the Selberg zeta function, Max-Planck-Insitut für Mathematik, Bonn, June 2002.

(Note these talks were given after the grant was submitted but before funding began.)

Peter Kleban, invited talk on 'SLE Crossing Probabilities and Modular Forms", at the workshop on Geometry and Statistics of Random Growth, Institut Henri Poincaré, Paris, March 2003.

J. Fiala, "Renormalization Group results for the Farey fraction spin chain", Rutgers Statistical Mechanics meeting, Rutgers University, May 2003.

<u>2003-2004</u>:

Peter Kleban, invited talk on "Thermodynamics of the Farey fraction spin chain", Koc University, Istanbul, November 2003.

Peter Kleban, invited talk on "Crossing probabilities and modular forms", Fachbereich Mathematik, Universität Clausthal, Germany, November 2003.

Peter Kleban, invited talk on "Thermodynamics of the Farey fraction spin chain", Mathematics Department, Rutgers University, March 2004.

J. Fiala, talk on "Thermodynamics of the Farey fraction spin chain", Fifth Annual Greater Boston Area Statistical Mechanics Meeting, Brandeis University, Oct. 18, 2003.

J. Fiala, talk on "Thermodynamics of extended Farey spin chains", Rutgers Statistical Mechanics meeting, Rutgers University, December 2003.

<u>2004-2005</u>:

Peter Kleban, invited talk on "Stochastic Löwner Evolution and 2-D Critical Phenomena", Mathematics Department, Rutgers University, November 2004.

Peter Kleban, talk on "Strange and unusual correlations in the Farey spin chain", Rutgers Statistical Mechanics meeting, Rutgers University, December 2004.

2005-2006:

Peter Kleban, invited talk on "The Farey fraction spin chain", Rutgers Statistical Mechanics meeting, Rutgers University, May 2005.

Peter Kleban, invited talk on "Crossing Probabilities and Modular Forms", School of Mathematical Sciences, University of Nottingham, November 2005.

Peter Kleban, invited talk on "The Farey fraction spin chain", School of Mathematical Sciences, Queen Mary, University of London, November 2005.

Peter Kleban, invited talk on "The Farey fraction spin chain", London Dynamical Systems Group workshop on "Symbolic Dynamics and Number Theory in Statistical Mechanics", Queen Mary, University of London, February 2006.

2006-2007:

Peter Kleban, invited talk on "The Farey fraction spin chain" at the London Mathematical Society Durham Symposium on Dynamical Systems and Statistical Mechanics University of Durham, Durham, England, July 2007.

Presentations after this date were supported under continuation Grant No. DMR-0536927.