BOOK OF ABSTRACTS

of the

International Workshop and Young Scientist School on Critical Phenomena and Phase Transition

CPPT17

A.I. Alikhanyan National Science Laboratory, Yerevan, Armenia

20-24 September 2017

http://cppt.am/



Welcome

The workshop "International Workshop and Young Scientist School on Critical Phenomena and Phase Transition" will be held September 20-24, 2017 in Yerevan, Armenia. Phase transitions in equilibrium and, in particular, in non-equilibrium continue to be an area of great interest to researchers in a range of fields, from statistical physics, through lattice field theory, to sociophysics. The present meeting is designed to expose the state of the art in this field as well as to provide a stage for discussions about current challenges and future directions. The workshop is devoted to the fundamental concepts of statistical physics and intended to communicate a basic understanding of the central concepts of the field. Additionally, the conference is put together on the occasion of the 65th birthday of Nerses Ananikyan who significantly contributed to this field on a broad range of problems. The topics of this year's conference accordingly cover a broad range from spin systems to macromolecules. In particular, it is focused on critical phenomena and phase transition, exact results for lattice models, conformal field theory, self-organized criticality, chaos and dynamical system, entanglement, complex network science.

Topics:

- Critical Phenomena and Phase Transition.
- Computational Physics and Numerical Simulation
- Exact Results for Lattice Models
- Conformal Field Theory

CPPT17







International Workshop and Young Scientist School on Critical Phenomena and Phase Transition

20-24 September 2017

A.I. Alikhanyan National Science Laboratory Yerevan, Armenia

Lecture Hall
L.A. Orbeli Institute of Physiology NAS RA
22 Orbeli Brothers St, Yerevan

Speakers

Armen Allahverdyan (Yerevan) Bertrand Berche (Nancy) Elmar Bittner (Heidelberg) Ruben Gulhazaryan (Yerevan) Tigran Hakobyan (Yerevan) Vahan Hovhannisyan (Yerevan) Wolfhard Janke (Leipzig) Gholamreza Jafari (Tehran) Desmond Johnston (Edinburgh) Yevgeni Mamasakhlisov (Yerevan) Vladimir Morozov (Yerevan) Vadim Ohanyan (Yerevan) Anna Okopińska (Kielce) Hayk Poghosyan (Yerevan) Rubik Poghossian (Yerevan) Vahagn Poghosyan (Yerevan)
Philippe Ruelle (Louvain)
David Saakian (Yerevan)
Afsaneh Sadrolashrafi (Yerevan)
Shushanik Tonoyan (Yerevan)
Reza Torabi (Tafresh)
Martin Weigel (Coventry)

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Wed, 20 September

09.00 - 09.45 Registration 09:45 - 10:00 Opening

Session chair: P. Ruelle

- **10.00 10.45 B. Berche** (*University de Lorraine, France*) Fermions in curved spacetime: how torsion may be used to manipulate spin.
- **10.45 11.15 E. Bittner** (*Heidelberg University*, *Germany*) On the interface tension of the Ising model.

11:15 - 11:45 Coffee Break

- **11:45 12:30 M. Weigel** (*Coventry Unversity, UK*) Population annealing: Massively parallel simulations in statistical physics.
- **12:30 13:00 T. Hakobyan** (Yerevan State University, Armenia) Lowest-energy states in SO(N) spin chain

13:00 - 15:00 Lunch Break

- 15:00 15:45 Y. Mamasakhlisov (Yerevan State University, Armenia) Reentrant Melting of Single - Stranded RNA with Quenched Sequence Randomness
- **15:45 16:15 V. Morozov** (Yerevan State University, Armenia) The helix-coil transition the frames of GMPC. Ligands effects.

17:30 Welcome party at Olympia hotel

Thu, 21 September

Session chair: M. Weigel

10:00 - 10:45 P. Ruelle (*Catholic University of Louvain, Belgium*) Variations on the discrete Laplacian.

10:45 - 11:15 V. Poghosyan (Institute for Informatics and Automation Problems, Armenia) Spiral Structures and Subdiffusion of the Rotor-Router Walk

11:15 - 11:45 Coffee break

- 11.45 12.30 D. Johnston (Heriot-Watt University, UK) SUSY, spin chains and ASEPS
- **12:30 13:00 Resa Torabi** (*Tafresh university, Iran*) Reaction-Superdiffusion Systems near the Hoph Instability

13.00 - 15.00 Lunch Break

- 15:00 15:30 A. Okopińska (Jan Kochanowski University, Poland) Entanglement on the border between bound and resonant states
- 15:30 16:00 V. Hovhannisyan (A.I. Alikhanyan National Science Laboratory, Armenia) Ensemble inequivalence in the mean-field Blume-Emery-Griffiths model.

16:30 Excursion to ARARAT cognac factory

Fri, 22 September

Session chair: D. Johnston

- **10:00 10:45 R. Poghosyan** (A.I. Alikhanyan National Science Laboratory, Armenia) Recurrence relations for the W_3 conformal blocks and N=2 SYM partition functions
- 10:45 11:15 D. Saakian (A.I. Alikhanyan National Science Laboratory, Armenia)

 The exact solution of the Hidden Markov processes and the product of correlated random matrices.

11:15 - 11:45 Coffee break

- **11.45 12.30 V. Ohanyan** (Yerevan State University, Armenia) Effects of non-conserved magnetization operator on the magneto-thermal properties of spin-clusters and chains.
- 12:30 13:00 H. Poghosyan (A.I. Alikhanyan National Science Laboratory, Armenia) Dynamical system approach and super-stable points for

antiferromagnetic spin-1 Ising-Heisenberg models on diamond chain and diamond-like decorated Bethe lattices.

13:00 - 14:00 Lunch Break

14:30 Excursion to Garni - Geghard

Sat, 23 September

Session chair: R. Poghosyan

- **10:00 10:45 W. Janke** (*Leipzig University, Germany*) Exact enumeration of self-avoiding walks on critical percolation clusters in two to seven dimensions.
- 10:45 11:15 R. Ghulhazaryan (A.I. Alikhanyan National Science Laboratory, Armenia) Numerical Study of Partition Function Zeros on Recursive Lattices.

11:15 - 11:45 Coffee break

- 11:45 12:30 A. Allahverdyan (A.I. Alikhanyan National Science Laboratory, Armenia) Stochastic Model for Phonemes Uncovers an Author-Dependency of Their Usage.
- 12:30 13:00 A. Sadrolashrafi (A.I. Alikhanyan National Science Laboratory, Armenia) Magnetization plateaus and thermal negativity in spin-1 Nicontaining polymer.

13.00 - 15.00 Lunch Break

- 15:00 15:30 G. Jafari (Shahid Beheshti University, Iran) Aged networks dynamics
- 15:30 16:00 Sh. Tonoyan (Yerevan State University, Armenia) Constrained annealing approach for order-disorder transitions in heterogeneous macromolecular systems
- 16:00 Closing remarks

18:00 Banquet in restaurant at Olympia hotel

Armen Allahverdyan (A.I. Alikhanyan National Science Laboratory, Armenia)

Bertrand Berche (University de Lorraine, France)

Elmar Bittner (Heidelberg University, Germany)

Ruben Ghulhazaryan (A.I. Alikhanyan National Science Laboratory, Armenia)

Tigran Hakobyan (Yerevan State University, Armenia)

Vahan Hovhannisyan (A.I. Alikhanyan National Science Laboratory, Armenia)

Wolfhard Janke (Leipzig University, Germany)

Gholamreza Jafari (Shahid Beheshti University, Iran)

Desmond Johnston (Heriot-Watt University, UK)

Yevgeni Mamasakhlisov (Yerevan State University, Armenia)

Vladimir Morozov (Yerevan State University, Armenia)

Vadim Ohanyan (Yerevan State University, Armenia)

Anna Okopińska (Jan Kochanowski University, Poland)

Hayk Poghosyan (A.I. Alikhanyan National Science Laboratory, Armenia)

Rubik Poghossian (A.I. Alikhanyan National Science Laboratory, Armenia)

Vahagn Poghosyan (Institute for Informatics and Automation Problems, Armenia)

Philippe Ruelle (Catholic University of Louvain, Belgium)

David Saakian (A.I. Alikhanyan National Science Laboratory, Armenia)

Afsaneh Sadrolashrafi (A.I. Alikhanyan National Science Laboratory, Armenia)

Shushanik Tonoyan (Yerevan State University, Armenia)

Resa Torabi (Tafresh university, Iran)

Martin Weigel (Coventry University, UK)

Stochastic Model for Phonemes Uncovers an Author-Dependency of Their Usage

Armen Allahverdyan¹ (with Weibing Deng²)

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Studying the hierarchic structure of language (phoneme, syllable, morpheme, word ...) can be inspired by methods employed for physical systems (atoms, molecules, ...). We study rank-frequency relations for phonemes, the minimal units that still relate to linguistic meaning. We show that these relations can be described by the Dirichlet distribution, a direct analogue of the ideal-gas model in statistical mechanics. This description allows us to demonstrate that the rank-frequency relations for phonemes of a text do depend on its author. The author-dependency effect is not caused by the author's vocabulary (common words used in different texts), and is confirmed by several alternative means.

W.Deng and A. Allahverdyan, PLoS ONE 11(4), e0152561 (2016).

Fermions in curved spacetime: how torsion may be used to manipulate spin

Bertrand Berche

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We address the problem of quantum particles moving on a manifold characterised by the presence of torsion along a preferential axis. In fact, such a torsion may be taylored by the presence of a single screw dislocation, whose Burgers vector measures the torsion amplitude. The problem, first treated in the relativistic limit describing fermions that couple minimally to torsion, is then analysed in the Pauli limit. We show [1] that torsion induces a geometric potential and also that it couples generically to the phase of the wave function, giving rise to the possibility of using torsion to manipulate spin currents in the case of spinor wave functions. These results emerge as an alternative strategy for using screw dislocations in the design of spintronic-based devices.

[1] S. Fumeron, B. Berche, E. Medina, F. Santos and F. Moraes, *Using torsion to manipulate spin currents*, EPL 117 (2017) 47007.

On the interface tension of the Ising model

Elmar Bittner

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We determine the interface tension for the two and three dimensional Ising model using multicanonical simulations. We analyse the finite-size scaling behaviour of the interface tension for various temperatures, and compare them to previous results obtained with a combination of the multimagnetic algorithm with the parallel tempering method. We also use exact finite-size scaling functions for the two dimensional Ising model to validate our results.

Numerical Study of Partition Function Zeros on Recursive Lattices

Ruben Ghulghazaryan

(with Nerses Ananikian)

A.I. Alikhanyan National Science Laboratory, Yerevan, Armenia ghulr@yahoo.com

A numerical method for investigation of complex zeros of the partition function of models with one-dimensional recurrence mapping on the Cayley-tree is developed. A generalized recurrence relation for partition function calculation is derived. It is shown that zeros of the partition function correspond to the set of external parameters (kT, magnetic field) for which the recurrence function has neutral periodical cycles. On the complex plane zeros of the partition function generate Mandelbrot-like sets with fractal structure. This phenomena is known as the universality of the Mandelbrot set of the quadratic mapping $z\rightarrow z^2+c$. On the other hand, the Yang-Lee zeros of multi-site interaction spin-1/2 Ising model in the presence of inhomogeneous magnetic field on the Cayley-type lattice is associated with the Julia set of the corresponding recurrence mapping and investigated.

Lowest-energy states in SO(N) spin chain

Tigran Hakobyan

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The symmetry of the open finite-size SO(N) spin chain is expanded to O(N) using the particle parities. It is proven that the lowest-energy states in eigenspaces, specified by theses parities, are nondegenerate and combined into antisymmetric tensors. At the valence-bond point all lowest states form a single highly degenerate ground state.

Ensemble inequivalence in the mean-field Blume-Emery-Griffiths model

Vahan Hovhannisyan¹

(with Alessandro Campa², Stefano Ruffo³ and Nerses Ananikian¹)

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We study the inequivalence of canonical and microcanonical ensembles in the mean-field BlumeEmery-Griffiths model [1]. In both ensembles the thermodynamic phase diagrams strongly depend on the value of the biquadratic exchange interaction. At small values, as for the Blume-Capel model, first and second order phase transitions between a ferromagnetic and a paramagnetic state are present. The location of the tricritical point, separating second order and first order transitions, differs in the two ensembles [2]. At higher values of the biquadratic exchange interaction, a further phase transition between two paramagnetic states with different values of the quadrupole moment appears. It is characterized by a critical point and its location is not the same in the two ensembles. Furthermore, we study ergodicity breaking [3]: gaps in the accessible values of magnetization are present at low energies.

- [1] M. Blume, V. J. Emery and R.B. Griffiths, Phys. Rev. A 4, 1071 (1971).
- [2] J. Barré, D. Mukamel and S. Ruffo, Phys. Rev. Lett. 87, 030601 (2001).
- [3] D. Mukamel, S. Ruffo, and N. Schreiber, Phys. Rev. Lett. 95, 240604 (2005).

Aged networks dynamics Gholamreza Jafari

Shahid Beheshti University, Tehran, Iran g_jafari@sbu.ac.ir

Evolution of social networks based on balance theory happens to reduce stress with the evolution of their links. Each link has to participate in this evolution without any excuse. But in the real systems the relationships are not mathematics parameter to change without any consideration. However, not all the links would need to evolve in such a process, there are some links with no tendency to change, because of their historical relationship. In other word, we have not forgot the old friends/enemies easily. In this presentation, I will show how sometimes memory is a threat to network stability of a network in the framework of social balance theory.

Exact enumeration of self-avoiding walks on critical percolation clusters in two to seven dimensions

Wolfhard Janke

(with Niklas Fricke)

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We study self-avoiding walks on critical percolation clusters by means of a recently developed exact enumeration method, which can handle walks of several thousand steps. We had previously presented results for the two- and three-dimensional cases; here we take a wider perspective and vary the system's dimensions up to D=7, beyond the supposed upper critical dimension of D_{uc} =6. These results may serve as a check of analytical predictions and help understand how the medium's fractal structure impacts on the walks' scaling behavior. For the physically relevant, smaller dimensions, the scaling exponent α for the end-to-end distance turns out to be smaller than previously thought and appears to be the same on the backbones as on full clusters. For the number of conformations, the "partition function", we find strong evidence against the widely assumed scaling law and propose an alternative, which perfectly fits our data.

N. Fricke and W. Janke, Phys. Rev. Lett. 113, 255701 (2014).

N. Fricke and W. Janke, J. Phys. A: Math. Theor. 50, 264002 (2017).

SUSY, spin chains and ASEPS

Desmond Johnston

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Supersymmetry (SUSY) is a symmetry originally proposed between odd and even spin particles in high energy particles physics which has so far stubbornly refused to appear. However, it has been found to exist in solid state physics in quantum spin chains where it appears to be closely related to exactly solvability. In spin chains SUSY relates chains of different length. In the Asymmetric exclusion process (ASEP) a "transfer matrix" symmetry also relates ASEP configurations of differing lengths. The similarities between these symmetries are intriguing we discuss investigating these using methods from the theory of integrable systems.

Reentrant Melting of Single - Stranded RNA with Quenched Sequence Randomness

Yevgeni Mamasakhlisov¹

(with A. Andreassian¹ and A. Hakobyan²)

¹Yerevan State University, Yerevan, Armenia ²The Institute of Radiophysics & Electronics, Ashtarak, Armenia y.mamasakhlisov@ysu.am

The effect of quenched sequence disorder on the thermodynamics of RNA secondary structure formation is investigated for two-letter alphabet models using the constrained annealing approach, from which the temperature behavior of the free energy, specific heat, and helicity is analytically obtained. For competing base pairing energies, the calculations reveal reentrant melting at low temperatures, in excellent agreement with numerical results. Our results suggest an additional mechanism for the experimental phenomenon of RNA cold denaturation.

The helix-coil transition the frames of GMPC. Ligands effects.

Vladimir Morozov

(with Aram Andriasyan, Saadat Mirtavoosi, Shushanik Tonoyan and Yevgeni Mamasakhlisov)

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Within the framework of the Generalized Model of the Polypeptide Chain (GMPC)((Hairyan, Ananikyan et al. (1990), (1990); Morozov et al. (2004)), we studied the effect of ligands interacting in various ways on the helix-coil transition. The most general case, where for each type of interaction, there are several sites for ligand or solvent molecules was considered. It has been shown that the model can be reduced to the base one by redefinition of energy and entropy parameters, and in contrast to the pure solvent case (Badasyan et al. (2014)) both parameters are affected by competitive and non-competitive interactions. As a result, the temperature behavior of the system in a two - component environment richer transitions compared to a single component. It was also shown that a change in the concentration of ligand in the solvent transition temperature varies monotonically from the transition point of pure solvent to the transition point of pure ligand according to the expression,

$$cf_L(t_m) + (1-c)f_S(t_m) = 0$$

where $f_S(t_{m_s})=0$ and $f_L(t_{m_L})=0$ are equations for definition of melting temperature for pure solvent and ligand correspondingly. Our results allow to explain the experimental results concerning the stabilization of polyalanine by polyethylene glycol (Koutsioubas et al. (2012)) at the microscopic level. Our theoretical results can be interpreted as follows. Water compete for hydrogen bond formation. Despite the fact that the ligand does not interact, but prevents this competition taking up space, leading to stabilization.

Sh.A. Hairyan, N.S. Ananikyan, E.Sh. Mamasakhlisov, and V.F. Morozov, *Helix-coil transition in polypeptides. Microscopic approach*. Biopolymers, 30, (1990) 357. Sh.A. Hairyan, E.Sh. Mamasakhlisov, and V.F. Morozov, *The helix-coil transition in polypeptides: a microscopic approach. II*. Biopolymers, 35(1), 75 (1995).

V.F. Morozov, A.V. Badasyan, A.V. Grigoryan, M.A. Sahakyan, and Y.Sh. Mamasakhlisov, *Stacking and hydrogen bonding: DNA cooperativity at melting*. Biopolymers, 75, 434 (2004).

A.V. Badasyan, Sh. A. Tonoyan, Giacometti, A., R. Podgornik, V.A. Parsegian, Y. Sh. Mamasakhlisov, and V. F. Morozov, *Unified description of solvent effects in the helix-coil transition*. Phys. Rev. E 89, 022723 (2014).

A. Koutsioubas, D. Lairez, S. Combet, G. C. Fadda, S. Longeville, and G. Zalczer, *Crowding effect on helix-coil transition: beyond entropic stabilization*. Journal of Chemical Physics 136, 215101 (2012).

Effects of non-conserved magnetization operator on the magneto-thermal properties of spin-clusters and chains.

Vadim Ohanyan

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We examine the general features of the non-commutativity of the magnetization operator and Hamiltonian for small quantum spin clusters. The source of this non-commutativity can be a difference in the Landé g-factors for different spins in the cluster, XY-anisotropy in the exchange interaction and the presence of the Dzyaloshinskii-Moriya term in the direction different from the direction of the magnetic field. As a result, zero-temperature magnetization curves for small spin clusters mimic those for the macroscopic systems with the band(s) of magnetic excitations, i.e. for the given eigenstate of the spin cluster the corresponding magnetic moment can be an explicit function of the external magnetic field yielding the nonconstant (non-plateau) form of the magnetization curve within the given eigenstate. In addition, the XY-anisotropy makes the saturated magnetization (the eigenstate when all spins in cluster are aligned along the magnetic field) inaccessible for finite magnetic field magnitude (asymptotical saturation). We demonstrate all these features on three examples: spin-1/2 dimer, mixed spin-(1/2,1) dimer, spin-1/2 ring trimer. We consider also the simplest Ising-Heisenberg chain, the Ising-XYZ diamond chain with four different g-factors. In the chain model the magnetization curve has a more complicated and non-trivial structure which that for clusters.

Entanglement on the border between bound and resonant states

Anna Okopińska

Jan Kochanowski University, Poland okopin@fuw.edu.pl

Studying the physics of quantum correlations has gained increasing attention since the first experimental fabrication of artificial few-body systems on the nanoscale, such as semiconductor quantum dots or small ensembles of ultracold atoms in optical traps. Those structures may be considered as composed of a small number of interacting elements with controllable and highly tunable parameters, effectively described by Schrödinger equation. Performing analytical and numerical studies of simple models of few-body systems over a broad range of their parameters may provide a deeper understanding of correlation effects, especially in the neighborhood of critical points.

Bipartite correlations are well characterized by the entanglement spectrum, i.e. the eigenvalues of the reduced density matrix of the system partitioned into two subsystems. Entropies of entanglement spectrum can be conveniently used as correlation measures. I will study the entanglement spectrum of different few-body systems where the interactions depend on various powers of the distance between the constituents. Both closed and open systems will be considered. The linear entropy and von Neumann entropy will be discussed in dependence on the interaction type and strength. Particular attention will be paid to the behavior of entanglement on the border between the regimes of bound and resonant states.

Recurrence relations for the W₃ conformal blocks and N=2 SYM partition functions

Rubik Poghossian

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Recursion relations for the sphere 4-point and torus 1-point W3 conformal blocks, generalizing Alexei Zamolodchikov's famous relation for the Virasoro

conformal blocks are proposed. The first relation is valid for any 4-point conformal block with two arbitrary and two special primaries with charge parameters proportional to the highest weight of the fundamental irrep of SU(3). The other relation is designed for the torus conformal block with a special (in above mentioned sense) primary field insertion. AGT relation maps the sphere conformal block and the torus block to the instanton partition functions of the N=2 SU(3) SYM theory with 6 fundamental or an adjoint hypermultiplets respectively. AGT duality played a central role in establishing these recurrence relations, whose gauge theory counterparts are novel relations for the SU(3) partition functions with Nf=6 fundamental or an adjoint hypermultiplets. By decoupling some (or all) hypermultiplets, recurrence relations for the asymptotically free theories with $0 {\le} N_f < 6$ are found.

Dynamical system approach and super-stable points for antiferromagnetic spin-1 Ising-Heisenberg models on diamond chain and diamond-like decorated Bethe lattices.

Hayk Poghosyan

(with Nerses Ananikian)

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We consider the appearance of super-stable cycles in the dynamical approach to the antiferromagnetic and ferromagnetic spin-1 Ising and Ising-Heisenberg models on a diamond chains and diamond-like decorated Bethe lattices. The rational mappings, which provide statistical properties of the model, are derived by using recurrence relation technique.

For both models the results show a connection between magnetization plateaus and dynamical properties, as the behavior of Lyapunov exponents and super-stable cycles. The exact conditions for the existence of super-stable points are extracted.

Spiral Structures and Subdiffusion of the Rotor-Router Walk

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(with Vl.V. Papoyan^{2,3} and V.B. Priezzhev²)

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The rotor-router model on a graph describes a discrete-time walk accompanied by the deterministic evolution of configurations of rotors randomly placed on vertices of the graph. A rotor at a given vertex is an arrow that is directed to one of its neighbors.

A recurrent state of the rotor-routing process on a finite sink-free graph can be represented by a unicycle that is a connected spanning subgraph containing a unique directed cycle. We distinguish between short cycles of length 2 called "dimers" and longer ones called "contours". Then the rotor-router walk performing an Euler tour on the graph generates a sequence of dimers and contours which exhibits both random and regular properties. Imposing initial conditions randomly chosen from the uniform distribution of unicycles (USU) we calculate expected numbers of dimers and contours and correlation between them at two successive moments of time in the sequence. In addition, we analyze the mean-square displacement of the rotor-router walker (diffusive and sub-diffusive behaviors) for various initial states (USU and randomly directed rotors) and geometries (finite torus, infinite lattice, semi-infinite cylinder).

We show that the average width of the surface region of the visited sites (cluster) evolves with time to the stationary value by a scaling law whose parameters are close to the standard KPZ exponents. We introduce characteristic labels corresponding to closed clockwise contours formed by rotors and conjecture that the sequence of labels has an Archimedean property (spiral structure on the infinite square lattice, and helix structure on the semi-infinite cylinder).

- [1] Vl.V. Papoyan, V.S. Poghosyan and V.B. Priezzhev, *A loop reversibility of the rotor-router walk*, J. Phys. A: Math. Theor. 48, 285203 (2015).
- [2] Vl.V. Papoyan, V.S. Poghosyan and V.B. Priezzhev, *Spiral Structures in the Rotor-Router Walk*, J. Stat. Mech., 043207 (2016).

[3] Vl.V. Papoyan, V.S. Poghosyan and V.B. Priezzhev, *Rotor-Router Walk on a Semi-infinite Cylinder*, J. Stat. Mech., 073209 (2016).

Variations on the discrete Laplacian

Philippe Ruelle

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We will review some recent developments concerning the combinatorics of spanning trees, spanning forests and other related geometric structures. Applications of these will be discussed.

The exact solution of the Hidden Markov processes and the product of correlated random matrices.

David Saakian

A.I. Alikhanyan National Science Laboratory, Yerevan, Armenia saakian@phys.sinica.edu.tw

We write a master equation for the distribution of the product of random matrices, then deduce a functional equation for the master. We write a master equation for the distributions, related to Hidden Markov processes (HMP) and solve it using a functional equation. The latter for a general case can be solved only numerically. We derived exact expression for the limiting distribution of the words in HMP and entropy. Our expression for the entropy is alternative to the ones given before by the solution of integral equations. The exact solution is possible because actually the model can be considered as a generalized random walk on 1-d strip

Magnetization plateaus and thermal negativity in spin-1 Ni-containing polymer.

Afsaneh Sadrolashrafi

(with Nerses Ananikian)

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The experimental data of spin-1 Ni-containing polymer [Ni (NN'-dmen)(μ -N₃)₂]n was observed in [1]. The nitrogen μ -azido may give end-to-end (EE) or end-on (EO) coordination modes, where normally, the first one cause antiferromagnetic coupling and the latter would result in ferromagnetic coupling. From experiment, antiferromagnetic (AF) coupling is sufficiently large (J₃=-120 cm⁻¹) and ferromagnetic couplings are J₁=20cm⁻¹ and J₂=37 cm⁻¹. Magnetization plateaus occur both in antiferromagnetic and ferromagnetic materials and they play a great role in understanding of a large family of nontrivial quantum phenomena. We find out the behavior of the magnetization curves, magnetic susceptibility and thermal negativity.

[1] J. Ribas, et. al., Coord. Chem. Rev. 93 (1999); J. Ribas, et. al. Angew. Chem. Int. Ed. Engl. 35 (1996)

Constrained annealing approach for order-disorder transitions in heterogeneous macromolecular systems

Shushanik Tonoyan

(with A. Andreassian¹, A. Hakobyan², V.F. Morozov¹ and Y.Sh. Mamasakhlisov¹)

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Theory of helix-coil transition in heterogeneous biopolymers has been constructed on the base of the GMPC model using the constrained annealing approach, developed by M. Serva and G. Paladin (1993). An expression for the free energy of the heteropolymer has been obtained by averaging the transfer matrix of homopolymeric GMPC with redefined energy and conformational parameters. An algorithm for calculation of the melting curve of heteropolymeric system was obtained. The melting

curves of homopolymeric and heteropolymeric systems were compared. It was shown that the sequence heterogeneity qualitatively defines the main melting properties of random heteropolymer. It was shown that the melting interval is wider than for homopolymer. The melting temperature approximately is the linear function of homopolymer's melting temperature.

Reaction-Superdiffusion Systems near the Hoph Instability

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Self-organized phenomena are ubiquitous in nature especially in living systems [1]. They occur in open systems out of equilibrium and they have attracted the attention of scientists in different fields of science. Reaction-diffusion systems are extensively used in the study of self-organized phenomena [2]. They are sets of coupled partial differential equations which include diffusion terms and are useful in many fields such as biology, ecology neuroscience, physics and chemistry. As a matter of fact adding a diffusion term to a reaction system can drive the system to instability and plays an important role in the formation of spatio-temporal patterns out of equilibrium [3]. The characteristic feature of most of the studied reaction-diffusion systems is that the diffusion is normal. However, experimental evidences show that anomalous diffusion arises more frequently in nature [4]. This fact motivated us to consider anomalous diffusion in reaction-diffusion systems.

Here we study the effect of Levy superdiffusion on the instability of a general n-component reaction-superdiffusion system near the Hopf instability. Superdiffusion can be considered in reaction-diffusion systems using the powerful tool of fractional calculus. Utilizing the reductive perturbation theory we show that for a general n-component reaction-superdiffusion system, a universal fractional complex Ginzburg-Landau equation emerges as the amplitude equation near the Hopf instability. To illustrate the effect of superdiffusion we solve the fractional complex Ginzburg-Landau equation numerically. We use pseudospectral method to perform numerical computations in Fourier space. Numerical results indicate that the fractional order shifts the boundary of different regimes. As a result, superdiffusion introduces a new parameter that changes the dynamical properties of the system near the Hoph instability.

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Population annealing: Massively parallel simulations in statistical physics

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While Moore's law of semiconductors has ensured for over forty years that the next generation of processors works significantly faster than the current one, for the last ten years or so serial code has not seen any speed-up from new hardware which, instead, achieves performance improvements only from packing more and more cores onto a single die. As a consequence, scientists working with computer simulations need to move away from intrinsically serial algorithms to find new approaches that can make good use of potentially millions of computational cores. Population annealing, that was initially suggested by Hukushima and Iba and more recently was studied systematically by Machta, is a sequential Monte Carlo scheme that is potentially able to make use of such highly parallel computational resources. Additionally, it promises to allow for the accelerated simulation of systems with complex free-energy landscapes, much alike to the much more well known replica-exchange or paralleltempering approach. The relative performance with respect to such more traditional techniques, the appropriate choice of population sizes, temperature protocols and other parameters, the estimation of statistical and systematic errors and many other features, however, are essentially uncharted territory. Here, we use a systematic comparison of population annealing to Metropolis as well as parallel-tempering simulations for the Ising model to gauge the potential of this new approach, and we suggest a range of heuristics for its application in more general circumstances.

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From Olympia hotel to conference hall at Institute of Physiology



From airport to hotel Olympia

