

# MECO 39



## 39th Conference of the Middle European Cooperation in Statistical Physics

*8-10 April 2014, Coventry, England*



## Preface

This year marks the 40th anniversary of the first MECO conference. The *Middle European Cooperation in Statistical Physics* was founded during the Cold War as a series of international conferences aimed specifically at promoting open scientific dialogue and maintaining cooperation across Europe, despite the Iron Curtain. From its early days, MECO has grown to become one of Europe's most prestigious scientific forums in physics. It nowadays attracts the attention of a much wider academic community due to the broad nature of interdisciplinary applications of statistical physics. It has also grown geographically and has been hosted in many countries — including some not quite at in the physical middle of Europe.

Statistical physics is a major theme of Coventry University's Applied Mathematics Research Centre and we are pleased to host the conference for the first time in the UK. More than 100 participants from 20 countries are expected for MECO39, representing the continued vibrancy of our subjects. The Conference is organized in its traditional form of invited lectures (about 40 min.), oral contributions (about 20 min.) and poster presentations. The scope of the conference is wide, covering different fields of statistical mechanics and condensed matter physics, including soft matter, complex systems, networks, non-equilibrium and quantum systems as well as phase transitions and critical phenomena.

We are grateful for the kind sponsorship of a number of prestigious academic bodies and leading international journals (listed on page 9). We thank you for participating and we warmly welcome you to the ancient city of Coventry.

Coventry, March 2014

Christian von Ferber  
Damien Foster  
Nikolaos Fytas  
Nikolay Izmailian  
Ralph Kenna  
Thierry Platini  
Martin Weigel  
Taras Yavors'kii



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## Previous MECO conferences

1974 Wien (A)	1975 Regensburg (FRG)
1976 Bled (Y)	1977 Unterägeri (CH)
1978 Boszkowo (PL)	1979 Trieste (I)
1980 Budapest (H)	1981 Saarbrücken (FRG)
1982 Wien (A)	1983 Bled (Y)
1984 Gernrode (GDR)	1985 Aussois (F)
1986 Liblice (CS)	1987 Poidoux-Chexbres (CH)
1988 Karpacz (PL)	1989 Siena (I)
1990 Balatonfüred (H)	1991 Duisburg (D)
1994 Smolenice (SK)	1995 Puchberg/Wels (A)
1996 Bled (SL)	1997 Szklarska Poreba (PL)
1998 Trieste (I)	1999 Lutherstadt-Wittenberg (D)
2000 Pont-a-Mousson (F)	2001 Prague (CZ)
2002 Sopron (H)	2003 Saarbrücken (D)
2004 Bratislava (SK)	2005 Cortona (I)
2006 Primosten (CR)	2007 Ladek Zdroj (PL)
2008 Puchberg/Wels (A)	2009 Leipzig (D)
2010 Pont-a-Mousson (F)	2011 Lviv (UA)
2012 Tatrianske Matliare (SK)	2013 Trieste (I)

## International Advisory Board

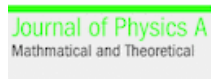
B. Berche (Nancy)  
K. Binder (Mainz)  
A. Cuccoli (Firenze)  
C. Di Castro (Roma)  
R. Folk (Linz)  
M. Henkel (Nancy)  
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## Sponsors





## Conference Schedule

## Tuesday, April 8

08:30 – – Registration and Wake-up Coffee – ☕  
09:15

09:15 – – Welcome & Opening –  
09:30

**Session 1: Slow Dynamics (Chair: Michael Allen)**

09:30 – **Leticia** Fast and slow quenches across second order  
10:10 **Cugliandolo** phase transitions: the density of topological  
defects

10:10 – **Juan Garrahan** Dynamical large deviations and glass transi-  
10:30 tions

10:30 – **Géza Ódor** Ageing of the 2+1 dimensional Kardar-Parisi-  
10:50 Zhang model

10:50 – – Coffee Break – ☕  
11:20

**Session 2: Disordered Systems (Chair: Michael Moore)**

11:20 – **Helmut** Self-organized criticality in Hamiltonian spin  
12:00 **Katzgraber** systems: ordinary, but intriguing

12:00 – **Ian Campbell** The critical properties of Ising Spin Glasses in  
12:20 dimensions five and four

12:20 – **Victor** Taming extreme fluctuations in spin glasses:  
13:00 **Martin-Mayor** temperature chaos and magnetic fields

13:00 – – Lunch – 🍽️  
14:00

14:00 –  
15:30

– **Poster Session I** –

**Session 3: Critical Phenomena (Chair: Wolfhard Janke)**

15:30 – **Anastasios** Parallel tempering and spin glasses  
16:10 **Malakis**

16:10 – **Richard Vink** Non-Ising critical point in a fluid with short-  
16:30 ranged interactions

16:30 – **Felix Höfling** Dynamic scaling and superdiffusion in a criti-  
16:50 cal binary mixture

16:50 – **Ferenc Iglói** Corner contribution to cluster numbers  
17:10

17:10 –  
17:40

– **Coffee Break** – ☕

**Session 4: Geometric Transitions (Chair: Katarina Uzelac)**

17:40 – **Nikolai** Monte Carlo study of jamming and percolation  
18:20 **Lebovka** of extended objects on lattices

18:20 – **Antonio** Crumpling transition on a crystalline mem-  
18:40 **Gordillo-**brane  
**Guerrero**

18:40 – **Des Johnston** Non-standard finite-size scaling at first-order  
19:00 phase transitions

## Wednesday, April 9

08:45 –  
09:30 – **Wake-up Coffee** – ☕

### Session 5: Foundations and Fluctuations I (Chair: Bertrand Berche)

09:30 – **Christian Maes** Nonequilibrium seas  
10:10

10:10 – **David Lopes** The critical Casimir force in a magnetic system: an experimental protocol  
10:30 **Cardozo**

10:30 – **Paola** Quantum environment for longer coherence time  
10:50 **Verrucchi**

10:50 – **Elzbieta** Wave function engineering in quantum nano-structures  
11:10 **Zipper**

11:10 –  
11:40 – **Coffee Break** – ☕

### Session 6: Polymers and Biophysics (Chair: Steffen Trimper)

11:40 – **Martin Evans** Speed selection in coupled Fisher waves  
12:20

12:20 – **Franco Ferrari** Polymer knots and links: Some experimental, analytical and numerical results  
12:40

12:40 – **Yurij** Variety of scaling laws for DNA denaturation  
13:00 **Holovatch**

13:00 –  
13:20 – **Conference Photo** –

13:30 –  
14:30 – **Lunch** – 🍽️

14:30 –  
22:30 – **Excursion to Stratford upon Avon** –

## Thursday, April 10

08:45 –  
09:30 – **Wake-up Coffee** – ☕

### Session 7: Soft Matter (Chair: Joseph Indekeu)

09:30 – **Thomas** Self organized dynamics of modular micro-  
10:10 **Palberg** swimmers

10:10 – **Slobodan** Knotty nematic fields  
10:50 **Žumer**

10:50 –  
11:20 – **Coffee Break** – ☕

### Session 8: Computational Physics (Chair: Elmar Bittner)

11:20 – **Lev Shchur** Towards Exaflops Monte Carlo computing  
12:00

12:00 – **David Saad** Planes, trains and polymers — the statistical  
12:20 physics of routing

12:20 – **Francesco** Entanglement spectra of interacting fermions  
12:40 **Parisen Toldin** in quantum Monte Carlo simulations

13:00 –  
14:00 – **Lunch** – 🍽️

### Session 9: Foundations and Fluctuations II (Chair: Yuriy Holovatch)

14:00 – **Stefan** Entropy for complex systems  
14:40 **Thurner**

14:40 – **Rosemary** Current fluctuations beyond one dimension:  
15:00 **Harris** subtleties and symmetries

15:00 –  
15:30 – **Coffee/Beer/Wine Break** – ☕

15:30 –  
17:00 – **Poster Session II** –

**Session 10: Quantum Systems (Chair: Ferenc Iglói)**

- 17:00 – **Rudolf Römer** Self-assembling tensor networks and holography in disordered spin chains  
17:40
- 17:40 – **Dragi Karevski** Driven Heisenberg spin chain with arbitrary boundary twisting angle: Exact results  
18:00
- 18:00 – **Alexandre** Decoherence in the central spin model  
18:20 **Faribault**





## List of Contributions

Seyma Akkaya Deviren	The crystal field effects for the Ising bilayer system consisting of spin-1/2 and spin-3/2
Nicolas Allegra	Partition function of the monomer-dimer model
Muhammad Anwar	Crystallization mechanism in melts of short n-alkane chains
Oscar Barbosa	Irreversibility by competition for a Glauber-Ising model by means of the entropy production
Elmar Bittner	MuCa vs WL: A tight race
Ian Campbell	The critical properties of Ising Spin Glasses in dimensions five and four
Massimo Cavallaro	Current fluctuations in a temporally correlated zero-range process
Levon Chakhmakhchyan	PageRank model of opinion formation on Ulam networks
Ben Collyer	Non-equilibrium steady states of Fokker-Planck-Boltzmann equation
Federico Corberi	Condensation of large fluctuations in a thermodynamical system
Leticia Cugliandolo	Fast and slow quenches across second order phase transitions: the density of topological defects
Silvio Dahmen	The Navajo and Quiche myths: a comparative study on the mythology of Amerindians

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Burçin Danacı	Evolved model regulatory networks form meta-networks in genotype and phenotype space
Bayram Deviren	Dynamic phase transitions in a cylindrical Ising nanowire
Sven Dorosz	Influence of random pinning on the crystallization process in suspensions of hard spheres
Eren Metin Elçi	Fragmentation of Potts clusters
Martin Evans	Speed selection in coupled Fisher waves
Alexandre Faribault	Decoherence in the central spin model
Michael Faulkner	Deconfinement and topological-sector fluctuations at the Berezinskii-Kosterlitz-Thouless phase transition
Franco Ferrari	Polymer knots and links: Some experimental, analytical and numerical results
Emilio J. Flores-Sola	Hyperscaling above the upper critical dimension in Ising models with long range interactions
Florian Günther	Structure optimization of BLN protein models combining local-search, evolutionary, and genetic approaches
Juan Garrahan	Dynamical large deviations and glass transitions
Antonio Gordillo-Guerrero	Crumpling transition on a crystalline membrane
Vyacheslav Gorev	Nonequilibrium processes in the vicinity of hydrodynamic states
Felix Höfling	Dynamic scaling and superdiffusion in a critical binary mixture
Rosemary Harris	Current fluctuations beyond one dimension: subtleties and symmetries

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Masayuki Hase	Dynamics of spherical model with correlated noise
Yurij Holovatch	Variety of scaling laws for DNA denaturation
Vahan Hovhannisyan	Ground-state, magnetic and partition function zeros properties of the spin-1 Ising-Heisenberg model on a diamond chain
Anja Humpert	Modelling of topological defects entangled around nanoparticles of nematic liquid crystal colloids
Ferenc Igloi	Corner contribution to cluster numbers
Wolfhard Janke	From amorphous aggregates to polymer bundles: The role of stiffness on structural phases in polymer aggregation
Puibasset Joel	Adsorption of a simple fluid in a nanopore: influence of system and reservoir size on the intermediate states visited
Des Johnston	Non-standard finite-size scaling at first-order phase transitions
Robert Juhasz	Distribution of dynamical quantities in the contact process, random walks, and quantum spin chains in random environments
Jakub Jędrak	Cluster size distribution in the autocatalytic growth model
Dragi Karevski	Driven Heisenberg spin chain with arbitrary boundary twisting angle: Exact results
Helmut G. Katzgraber	Self-organized criticality in Hamiltonian spin systems: ordinary, but intriguing
Hamid Khoshbakht	On the uniform sampling of ground states in the 2D $\pm J$ Ising spin glass model

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Istvan Kovacs	Corner contribution to percolation cluster numbers in three dimensions
Mariana Krasnytska	Lee-Yang-Fisher zeros for the Ising model on complex networks
Darka Labavic	A simple mechanism for controlling oscillations in coupled genetic circuits
Nikolai Lebovka	Monte Carlo study of jamming and percolation of extended objects on lattices
Chang-You Lin	Capillary wave and dynamical interfacial tension for a two-component Bose-Einstein condensate in strong segregation: I. Planar limit
David Lopes Cardozo	The critical Casimir force in a magnetic system: an experimental protocol
Krystyna Lukierska-Walasek	Statistical distributions and the entropy considerations in genetics
Christian Maes	Nonequilibrium seas
Anastasios Malakis	Parallel tempering and spin glasses
Krzysztof Malarz	Competing contact processes in the Watts–Strogatz network
Victor Martin-Mayor	Taming extreme fluctuations in spin glasses: temperature chaos and magnetic fields
Davide Michieletto	Threading dynamics of ring polymers in a gel
Olesya Mryglod	Aging of downloads of scientific publications: a case study
Davide Nuzzi	Manipulating qubits by spin chain soliton excitations
Geza Odor	Ageing of the 2+1 dimensional Kardar-Parisi-Zhang model
Guilherme Oliveira	Thermalization of low-dimensional quantum systems

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Thomas Palberg	Self organized dynamics of modular micro-swimmers
Francesco Parisen Toldin	Entanglement spectra of interacting fermions in quantum Monte Carlo simulations
Saete Pianegonda	Contact processes with competitive dynamics in bipartite lattices: effects of distinct interactions
Thierry Platini	Exact protein distributions for stochastic models of gene expression using partitioning of Poisson processes
Gergő Roósz	Evolution of the magnetization after a local quench in the critical transverse-field Ising chain
Rudolf A Roemer	Self-assembling tensor networks and holography in disordered spin chains
Rudolf A Roemer	Controlled engineering of extended states in disordered systems
Rudolf A Roemer	Multifractal finite-size-scaling and universality at the Anderson transition
Rudolf A Roemer	Localisation and finite-size effects in graphene
David Saad	Planes, trains and polymers — the statistical physics of routing
Stefan Schnabel	Sampling low energy states of the Edwards-Anderson model
Lev Shchur	Towards Exaflops Monte Carlo computing
Yair Shokef	Jamming percolation in three dimensions
Jacob Stevenson	Superposition enhanced nested sampling
Jozef Strecka	Magnetization process of the spin-1/2 Ising-Heisenberg and Heisenberg tetrahedral chain: a comparison
Stefan Thurner	Entropy for complex systems

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Steffen Trimper	Multiferroicity in doped and undoped BTO-nanoparticles
Paola Verrucchi	Quantum environment for longer coherence time
Yuri Vershinin	Road traffic flow modeling and signal optimisation for fuel economy and emissions reduction in Coventry City based on experimental data
Richard Vink	Non-Ising critical point in a fluid with short-ranged interactions
Pierre Wendenbaum	Entanglement via quantum repeated interactions
Benno Werlich	Specific interactions in a coarse-grained hard sphere model
Takuya Yamano	Gauge field for non-equilibrium processes and covariant version of Fisher information matrix
Joseph Yose	Network analysis of medieval texts: Case study of the Battle of Clontarf (1014 AD)
Yani Zhao	Thermal properties of polymer knots.
Elzbieta Zipper	Wave function engineering in quantum nanostructures
Marco Zoli	Path integral of twisted and bent DNA
Slobodan Zumer	Knotty nematic fields

## 11 – Fast and slow quenches across second order phase transitions: the density of topological defects

Leticia F. Cugliandolo

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When a dissipative macroscopic system is driven through a second order phase transition (a quench) it undergoes an ordering process, usually called phase ordering. During this process topological defects (be them domain walls, vortices or other) tend to disappear.

In this talk I will focus on the time and quench-rate dependence of the number density of topological defects in systems with scalar and vector order parameter. Typical examples of the former are Ising ferromagnets and of the latter are superfluids or superconductors. By combining scaling and numerical analysis I will show that the typical growing length of ordered regions determines the density of topological defects left over in the symmetry broken phase, far from the critical region, and that this is much lower than the one predicted by the Kibble-Zurek mechanism.

## 12 – Speed selection in coupled Fisher waves

Martin Evans

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The Fisher equation describes the spread of a population or the spread of an advantageous gene through a population. It is well known as a simple nonlinear equation which exhibits travelling wave solutions. Within statistical physics It has

played a major role in our understanding of phase ordering dynamics and random first order phase transitions. In this talk we review the selection mechanism for the speed of the travelling waves which was established some time ago. We go on to consider two coupled Fisher equations representing two populations e.g. sub-populations of bacteria which are susceptible or resistant to antibiotic. We show that a subtle coupling between two population waves gives rise to a novel speed selection mechanism.

[1] J. Venegas-Ortiz, R. J. Allen, and M. R. Evans, *Genetics*, vol. 196 (2014), 497.

## 13 – Self-organized criticality in Hamiltonian spin systems: ordinary, but intriguing

**Helmut G. Katzgraber**

Department of Physics and Astronomy, Texas A&M University  
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Self-organized criticality (SOC) refers to the tendency of dissipative systems to drive themselves into a scale-invariant critical state without any parameter tuning. These phenomena are of crucial importance because fractal objects displaying SOC are found everywhere, e.g., in earthquakes, the meandering of sea coasts, or in galactic clusters. Understanding its origin, however, represents a major unresolved puzzle. Pioneering work in the 1980s provided insights into the possible origins of SOC: The sandpile and forest-fire models are hallmark examples of dynamical systems that exhibit SOC. However, these models feature ad hoc dynamics, without showing how these can be obtained from an underlying Hamiltonian. The possible existence of SOC was also tested in random magnets, such as the random-field Ising model, but in all these, at least one parameter had to be tuned, i.e., no true SOC. The first Hamiltonian model displaying true SOC was the infinite-range mean-field Sherrington-Kirkpatrick spin-glass model. Here, we investigate the conditions required for general disordered magnets to display self-organized criticality. Our results are in disagreement with the traditional lore that self-organized criticality is a property of the mean-field regime of spin glasses. In fact, self-organized criticality is recovered only in the strict limit of a diverging number of neighbors. In light of these result, the behavior of damage spreading on scale-free networks, as well Coulomb glasses are discussed.



Work done in collaboration with Juan Carlos Andresen, Zheng Zhu, Yohanes Pramudya, Creighton K. Thomas, V. Dobrosavljevic, and Gergely T. Zimanyi.

- [1] Juan Carlos Andresen, Zheng Zhu, Ruben S. Andrist, Helmut G. Katzgraber, V. Dobrosavljevic, and Gergely T. Zimanyi, Phys. Rev. Lett. **111**, 097203 (2013).

## 14 – Monte Carlo study of jamming and percolation of extended objects on lattices

**Nikolai Lebovka<sup>1</sup>, Yuri Tarasevich<sup>2</sup>**

<sup>1</sup>Institute of Biocolloidal Chemistry named after F.D. Ovcharenko, NAS of Ukraine, 42, Boulevard Vernadskogo, 03142 Kiev, Ukraine

<sup>2</sup>Astrakhan State University, 20a Tatishchev Street, 414056 Astrakhan, Russia  
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The data of Monte Carlo simulation of jamming and percolation of the extended objects on lattices are reviewed. The extended objects can be represented by different specified geometries, e.g., linear k-mers (adjacent sites), kxk-squares, rectangles, and other. In the random sequential adsorption (RSA) model, the objects are deposited irreversibly, randomly and sequentially on the empty spaces and overlapping of objects is forbidden. This process continues up to attainment of the non-equilibrium jammed state when no further object can be deposited. In a general case, the objects can diffuse within near-neighbour sites (diffusion model, DRSA) or seek for a sufficiently large empty space all over the lattice (relaxation RRSA model). In the correlated deposition model (CA), some of extended objects (seeds) are initially deposited and then other extended objects are deposited along perimeters of the seeds or clusters. The review covers behaviour of the jamming concentration and percolation threshold versus the size and structure of extended objects for different models of deposition, partially oriented or completely disordered systems, and lattices with non-uniform structure.

## 15 – Nonequilibrium seas

Christian Maes

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Probes in weak contact with a nonequilibrium environment undergo an effective dynamics that does not need to satisfy the fluctuation-dissipation relation and for which the effective forces are not derived from a thermodynamic potential. The good news is that we start to understand these modifications and to see their systematics.

- [1] Christian Maes, On the Second Fluctuation-Dissipation Theorem for Nonequilibrium Baths, *Journal of Statistical Physics* 154, 705-722 (2014).

## 16 – Parallel tempering and spin glasses

Anastasios Malakis

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Parallel Tempering Monte Carlo simulations have been one of the major tools in Statistical Mechanics for the understanding of a variety of systems presenting rugged free-energy landscapes [1]. However, it is generally accepted that the efficiency and accuracy of the numerical scheme depend strongly on the chosen protocol, i.e., the temperature and replica-exchange selection methods. With this view in mind, in the first part of this talk, we present and test, using as measures specific heat errors and transfer efficiency of replicas, some parallel tempering protocols [2].

In the second part of the talk we review the outcome of a very recent Monte Carlo study of the  $\pm J$  Ising model in three-dimensions (3D) with a spatially uniaxially anisotropic bond randomness on the simple cubic lattice, including details of its phase diagram and universality aspects [3]. Finally, we discuss some preliminary results on the critical behavior of 2D and 3D spin-glass models in which the frustration (fraction of frustrated elementary squares) is continuously varied,

starting from the so-called “Mattis spin-glass” of zero frustration.

- [1] M.E.J Newman and G.T. Barkema, *Monte Carlo Methods in Statistical Physics* (Clarendon, Oxford, 1999).
- [2] A. Malakis and T. Papakonstantinou, Phys. Rev. E **88**, 013312 (2013).
- [3] T. Papakonstantinou and A. Malakis, Phys. Rev. E **87**, 012132 (2013).

## **17 – Taming extreme fluctuations in spin glasses: temperature chaos and magnetic fields**

**Victor Martin-Mayor**

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Spin glasses are deceptively simple model systems for complex behavior. In spite of continued efforts by the scientific community, many questions still remain open. These efforts include the building up of special purpose computers, such as the Janus machine, specifically designed for the simulation of spin glasses.

Here, we shall focus on two exotic features predicted long ago, but still controversial: temperature chaos and the presence of a glass transition in an externally applied magnetic field. The numerical investigation of both effects is hampered by rather extreme statistical fluctuations. The qualitatively different behavior from sample to sample renders the standard statistical analysis, based on sample averages, inadequate as a basis for a finite-size scaling study

By carefully considering extreme fluctuations in the Janus data set, we obtain clear results for both problems, as well as an understanding of the approach to the thermodynamic limit.

In particular, the presence of temperature chaos in three dimensional spin glasses is established [1]. We obtain as well an understanding of the relevant scaling laws (that were severely oversimplified in previous work).

As for the effects of an externally applied magnetic field, we show that the lack of scale invariance found in previous simulations is due to dramatic fluctuations. When these fluctuations are taken into account, scale invariance is recovered. In this way, we extrapolate the position of a possible critical temperature in a field (the so called de Almeida-Thouless line) [2]. These extrapolations are consistent with recent upper bounds obtained in non-equilibrium simulations [3], and

pinpoint the temperature regime where the would-be critical behavior should be observed. The problem becomes finally well posed. Therefore, one can hope that a few years from now, when we will have numerical access to lower temperatures, we will finally know whether there is a phase transition in a field, or not.

- [1] L.A. Fernandez, V. Martin-Mayor, G. Parisi, B. Seoane Europhysics Lett., **103**, 67003 (2013).
- [2] Janus Collaboration: M. Baity-Jesi et al., manuscript in preparation.
- [3] Janus Collaboration: M. Baity-Jesi et al., arXiv:1307.4998.

## 18 – Self organized dynamics of modular micro-swimmers

**Thomas Palberg**

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An elegant way of swimming at low Reynolds numbers is phoretic motion, which does not rely on any moving part. Rather, a self-generated gradient induces a relative motion between the swimmer surface and the immediately surrounding solvent. Depending on the type of generated gradient, this motion classifies as electro-, chemo-, or thermo-phoresis. Several fascinating experimental realizations have been demonstrated using individual compact swimmers of mainly rod or sphere type [1]. The approach to phoretic micro-swimming followed by our group is different in the sense, that our swimmers are modular objects [2]. Even the minimal modular swimmer consists of a reservoir particle releasing a local electrolyte gradient and the substrate providing a gradient driven electro-osmotic solvent flow (the motor) propelling the reservoir particle. Several reservoir particles organize to form schools, which show a schooling-swimming transition, once a single larger reservoir particle enters to take the lead. In fact the same effect is observed for any single reservoir particle and added inert colloidal particles taking the role of a gearing. Also other particles may be assembled by or attached to the reservoir particle carrying these along as cargo. Finally several ideas have been proposed to realize a convincing remote steering of the resulting complex [3]. None of the complex constituents shows any phoretic motion under isolated conditions. Propulsion here is an emergent property of the collective and cooperative self-organization into a dynamic complex. The talk will shortly sketch the present state in experimental

micro-swimming, explain the mechanisms behind and the challenges involved in realizing, understanding and optimizing modular micro-swimming and finish with an outlook on open issues.

- [1] W. Wang, W. Duan, S. Ahmed, T. E. Mallouk, A. Sen, *Nano Today* 8, 531-554 (2013).
- [2] A. Reinmüller, H. J. Schöpe, T. Palberg, *Langmuir* 29, 1738-1742 (2013).
- [3] T. Palberg, H. Schweinfurth, T. Köller, H. Müller, H. J. Schöpe, A. Reinmüller, *Eur. Phys. J. Special Topics* 222, 2835-2853 (2013).

## **19 – Self-assembling tensor networks and holography in disordered spin chains**

**Rudolf Römer, Andrew Goldsborough**

Department of Physics, University of Warwick, Coventry, CV4 7AL, UK

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We show that the numerical strong disorder renormalization group algorithm (SDRG) of Hikiyama et. al. [*Phys. Rev. B* 60, 12116 (1999)] for the one-dimensional disordered Heisenberg model naturally describes a tree tensor network (TTN) with an irregular structure dened by the strength of the couplings. Employing the holographic interpretation of the TTN in Hilbert space, we compute expectation values, correlation functions and the entanglement entropy using the geometrical properties of the TTN. We find that the disorder averaged spin-spin correlation scales with the average path length through the tensor network while the entanglement entropy scales with the minimal surface connecting two regions. Furthermore, the entanglement entropy increases with both disorder and system size, resulting in an area-law violation. Our results demonstrate the usefulness of a self-assembling TTN approach to disordered systems and quantitatively validate the connection between holography and quantum many-body systems [arXiv:1401.4874].

- [1] A. M. Goldsborough, R. A. Römer, "Self-assembling tensor networks and holography in disordered spin chains", submitted to *Phys. Rev. B* (2014).

# I10 – Towards Exaflops Monte Carlo computing

Lev Shchur

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Monte Carlo simulation is one of the main methods in Statistical Mechanics. We analyze current state of the research and development which goes toward the exaflops range of computing power for the Monte Carlo simulations. It is scalable Monte Carlo methods, new implementations for massive parallel computers, for hybrid supercomputers running GPGPU, parallel streams of random numbers, and other related topics.

# I11 – Entropy for complex systems

Stefan Thurner

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Shannon and Khinchin built their foundational information theoretic work on four axioms that completely determine the information-theoretic entropy to be of Boltzmann-Gibbs type,  $S_{BG} = -\sum_i p_i \log p_i$ . For non-ergodic systems the separation axiom (Shannon-Khinchin axiom 4) is not valid. We show that whenever this axiom is violated entropy takes the more general form,  $S_{c,d} \propto \sum_i^W \Gamma(d + 1, 1 - c \log p_i)$ , where  $c$  and  $d$  are characteristic scaling exponents, and  $\Gamma$  is the incomplete Gamma function. The exponents  $(c,d)$  parametrize equivalence classes which precisely characterise all (!) interacting and non-interacting statistical systems in the thermodynamic limit [1], including those that typically exhibit power laws or stretched exponential distributions. This allows us for example to derive Tsallis entropy (as a special case) from solid first principles. Further we show how the knowledge of the phase space volume of a system and the requirement of extensivity allows to uniquely determine  $(c,d)$ . We ask how these entropies are related to the 'Maximum entropy principle' (MEP). In particular we show how the first Shannon-Khinchin axiom allows us to separate the value for observing the most likely distribution function of a statistical system, into a 'maximum entropy' (log of multiplicity) and constraint terms. Remarkably, the generalized extensive

entropy is not necessarily identical with the generalized maximum entropy functional. In general for non-ergodic systems both concepts are tightly related but distinct. We demonstrate the practical relevance of our results on path-dependent random walks (non-Markovian systems with long-term memory) where the random walker's choices (left or right) depending on the history of the trajectory. We are able to compute the time dependent distribution functions from the knowledge of the maximum entropy, which is analytically derived from the microscopic update rules. Self-organized critical systems such as sand piles or particular types of spin systems with densifying interactions are other examples that can be understood within the presented framework.

- [1] R. Hanel, S. Thurner, A comprehensive classification of complex statistical systems and an axiomatic derivation of their entropy and distribution functions, EPL 93, 20006 (2011).
- [2] R. Hanel, S. Thurner, When do generalized entropies apply? How phase space volume determines entropy, EPL 96, 50003 (2011).
- [3] R. Hanel, S. Thurner, M. Gell-Mann, How multiplicity determines entropy. Derivation of the maximum entropy principle for complex systems, (in review 2014).

## I12 – Knotty nematic fields

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Complex geometrical constraints and intrinsic chirality lead to stable and metastable disclinations in nematic fields characterizing ordering in mesophases. The stabilization of these topological defects is a consequence of a balance between conflicting effects of confinement and chirality. Recently it was demonstrated that knots and links of arbitrary complexity can be formed with laser manipulation of disclinations entangling colloidal particles in nematic liquid crystals [1]. Understanding the stability, ordering, and assembly of such topological soft matter systems require a synergy of theory and simulations. In this overview I first describe our extension of the conventional topological theory of nematic defects by including the self-linking number as a topological invariant that enable classifying nematic disclination networks that include knots and links [2]. The approach will

be illustrated on numerically modeled nematic braids that were in partially also experimentally identified: knotted 2D nematic colloidal crystals [1], 3D opal structures permeated by nematics [3], knots in cholesteric droplets [4], and mutually tangled colloidal knots & defect loops in nematic fields [5].

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- [3] S. Čopar, N. A. Clark, M. Ravnik and S. Žumer, *Elementary building blocks of nematic disclination networks in densely packed 3D colloidal lattices*, *Soft Matter* **9** (2013) 8203.
- [4] D. Seč, S. Čopar and S. Žumer, *Topological zoo of free-standing knots in confined chiral nematic fluids*, *Nature Communications* **5** (2014) 3057.
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## Contributed Oral Presentations

## C1 – The critical properties of Ising Spin Glasses in dimensions five and four

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Extensive simulations are made on Ising Spin Glasses (ISG) with Gaussian and bimodal interaction distributions in dimensions five and four. A detailed explanation is first given of scaling with the natural ISG scaling variable  $\tau = 1 - \beta^2/\beta_c^2$  and the appropriate scaling expressions, which allow scaling analyses over the entire paramagnetic range of temperatures once the transition temperatures have been established using a combination of finite size scaling and of thermodynamic derivative peak data. Measurements in the thermodynamic limit regime are analysed in order to obtain estimates of the critical exponents and correction terms. The Privman-Fisher ansatz then leads to compact scaling expressions over the complete paramagnetic temperature range and for all sample sizes  $L$ . Comparisons between the Gaussian and bimodal ISGs show that the critical dimensionless parameters characteristic of a universality class, and the susceptibility and correlation length critical exponents  $\gamma$  and  $\nu$ , depend on the form of the interaction distribution. From these observations it can be deduced that critical exponents are not universal in ISGs, at least in these dimensions.

## C2 – Decoherence in the central spin model

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When using the spin of a single electron trapped in a quantum dot as an implementation of a qubit, its hyperfine coupling to the environmental nuclear spins ultimately leads to the decoherence of any prepared initial state. In this talk we will discuss how one can numerically exploit the quantum integrability of the Central Spin Model describing such a system to study its non-equilibrium dynamics. Using the Algebraic Bethe Ansatz in conjunction with a simple Monte Carlo sampling procedure, we study how the electron's spin coherence factor evolves with time due to the presence of the nuclear spin bath.

- [1] A. Faribault and D. Schuricht, Phys. Rev. B **88**, 085323 (2013).
- [2] A. Faribault and D. Schuricht, Phys. Rev. Lett. **110**, 040405 (2013).

## C3 – Polymer knots and links: Some experimental, analytical and numerical results

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The physics of polymer knots and links is a multidisciplinary subject. On one side, it is a playground for field theoretical techniques, like the renormalization group method and, more recently, for topological field theories. On the other side, the investigations of the statistical mechanics of polymer rings have also a feedback in field theories. Examples are a few progresses in treating field theories with constraints and a class of identities that allow to simplify complicated interactions in scalar field theories. Moreover, models of polymer knots and links have a range of applications that go beyond the physics of polymers and become relevant to other disciplines, in which the topological properties of quasi one-dimensional objects

play an important role. This is the case of magnetohydrodynamics and of some systems of quasiparticles with non-trivial statistics in solid state physics. Nowadays, the behavior of single polymer knots can be checked experimentally and it is possible to create polymer melts containing a very high percentage of polymer rings entangled together. Properties which are too difficult to be studied directly via experiments may be investigated thanks to reliable numerical simulations. In this introductory talk some of the recent experimental, analytical and numerical results in the physics of polymer knots and links will be presented.

## C4 – Dynamical large deviations and glass transitions

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The dynamics of many-body systems is often richer than what one can infer simply from their statics. This dynamical richness is revealed by considering strictly dynamical observables. The full statistical characteristics of such quantities encode the dynamical properties of the system at hand. By considering their large-deviations it is possible to derive a “statistical mechanics of trajectories”, which is to trajectories of the dynamics what equilibrium statistical mechanics is to configurations of the statics. In this talk I will describe this approach and how it can be applied to the glass transition problem. I will show that underlying kinetic phenomenon of glass formation is a novel class of order-disorder transitions in trajectory, rather than configuration, space. I will also discuss further implications of this large-deviation approach.

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- [2] L.O. Hedges, R.L. Jack, J.P. Garrahan and D. Chandler, Science 323, 1309 (2009).
- [3] C. Flindt and J.P. Garrahan, Phys. Rev. Lett. 110, 050601 (2013).
- [4] A.S. Keys, D. Chandler and J.P. Garrahan, arXiv:1401.7206.

## C5 – Crumpling transition on a crystalline membrane

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Antonio Gordillo-Guerrero<sup>2</sup>, Pedro Monroy<sup>3</sup>,  
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We study bidimensional triangular lattices with fixed connectivity, whose points are free to move in a 3D space. The hamiltonian of the system includes two terms: i) an elastic term of interaction between neighboring points, as if they were joined by a spring, ii) a curvature term of interaction between neighboring plaquettes, tending to put all plaquettes in the same plane. The strength of the latter is defined by a coupling constant called  $\kappa$ . For  $\kappa$  large, we expect an almost plane membrane, while for  $\kappa$  small we expect a crumpled surface. Therefore  $\kappa$  plays the role of the temperature as an external variable controlling the phase of the system.

In this work we estimate numerically the critical value of the coupling,  $\kappa_{c_1}$ , and the critical exponents of the observed phase transition. We compare with previous results on smaller systems [1] obtaining quite good agreement. We adapted the simulation codes for running in GPUs, obtaining a gain factor of 6 respect our simulations in CPUs. This work will presumably pave the way for simulations of more complex models including disorder, dilution or different geometries.

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## C6 – Dynamic scaling and superdiffusion in a critical binary mixture

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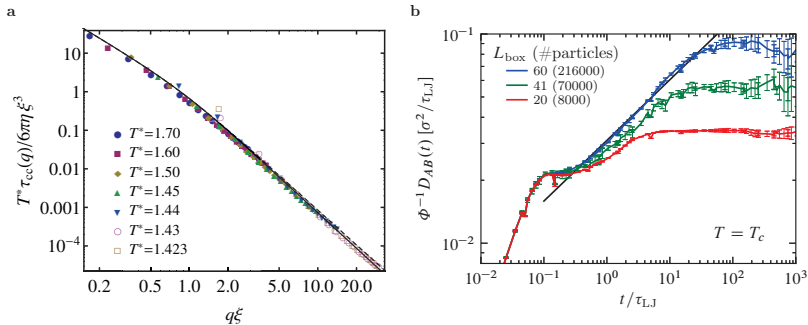
A binary mixture near its consolute point exhibits critical fluctuations of the local composition. The static properties of the mixture are well described by the 3D Ising universality class [1], the dynamic properties involving conservation of particles, energy, and momentum are classified as *model H'*. So far, theoretical work on the critical dynamics has focused on transport coefficients, while studies of the relaxation dynamics of the spatially resolved order parameter are missing.

We present numerical results for the dynamic structure factor  $S(k, t)$  of a symmetric binary Lennard-Jones mixture near its demixing transition. Employing the computing resources of high-end GPUs [2], we have performed microcanonical molecular dynamics simulations which cover system sizes of up to 216,000 particles and 4 non-trivial orders of magnitude in time. We explore the crossover of the  $k$ -dependent relaxation time from diffusion-like to critical behaviour and find nice agreement with theoretical predictions. Dynamic scaling of  $S(k, t)$  at criticality is tested and scaling functions are deduced.

For interdiffusion, we present a scaling argument and numerical evidence that the vanishing of the diffusion constant is accompanied by *superdiffusion* within a growing time window. Such behaviour is forbidden in purely relaxing systems and crucially depends on the presence of inertia.

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a) Scaling of the relaxation times  $\tau_{cc}(q)$  for a series of temperatures approaching the critical one,  $T_c^* \approx 1.423$ . b) Superdiffusive growth of the interdiffusion coefficient  $D_{AB}(t)$  at criticality for different sizes of the simulation box.

## C7 – Current fluctuations beyond one dimension: subtleties and symmetries

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Non-equilibrium steady states are characterized by currents of particles or energy whose large deviation properties can reveal symmetries and phase transitions. Here I will discuss some results on current fluctuations in interacting particle systems with open boundaries and topologies beyond one-dimension. In particular, I will present an anisotropic generalization of the recently proposed Isometric Fluctuation Relation [1] and test its validity for the paradigmatic zero-range process using both exact and fluctuating hydrodynamic approaches. This contribution is based on joint work published in [2, 3].

- [1] P. I. Hurtado, C. Pérez-Espigares, J. J. del Pozo, and P. L. Garrido, Proc. Natl. Acad. Sci. (U.S.A.) **108** (2011) 7704.
- [2] R. Villavicencio-Sanchez, R. J. Harris, and H. Touchette, J. Stat. Mech. **2012** (2012) P07007.
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## **C8 – Variety of scaling laws for DNA denaturation**

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Here, we rediscuss the thermal denaturation transition of DNA in a solvent: as the temperature is increased the DNA double strand separates into two individual single strands in an unbinding transition (also called denaturation transition). The discussion of the order of this transition has a long history ever since a minimal model was suggested by Poland and Scheraga. There are numerous studies devoted to determining the order of the transition between denaturated and bound DNA states. We briefly review some of the approaches and further discuss in detail the effects of the environment (quality of the solution, disorder) that may impact on the order of the transition. These show up in changes of the scaling exponents governing the conformational properties of DNA strands.

To this end, we re-consider the Poland-Scheraga model and apply a polymer field theory approach to calculate entropic exponents associated with the denaturated loop distribution. We discuss in particular variants of this transition that may occur due to the properties of the solution and that affect the self- and mutual interaction of both single and double strands.

We show that different environments may shift the transition towards or away from the first order regime. We find that the effects studied significantly influence the strength of the first order transition. This becomes manifest in the changes shown by the scaling laws that govern the DNA loop and strand distribution. As a

quantitative measure of these changes we present the values of the corresponding scaling exponents. In the 2D case exact exponents may be deduced, mapping the polymer model onto a two-dimensional random lattice modelling quantum gravity. For the 3D case we derive an expansion in  $4 - \varepsilon$  dimensions and evaluate the perturbation series to  $\varepsilon^4$  by means of resummation techniques.

This work is supported by FP7 Marie Curie Action grants PIRSES-GA-2011-295302-SPIDER and PIRSES-GA-2010-269139 - DCP-PhysBio

## C9 – Corner contribution to cluster numbers

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For the two-dimensional  $Q$ -state Potts model at criticality, we consider Fortuin-Kasteleyn and spin clusters and study the average number  $N_\Gamma$  of clusters that intersect a given contour  $\Gamma$ . To leading order,  $N_\Gamma$  is proportional to the length of the curve. Additionally, however, there occur logarithmic contributions related to the corners of  $\Gamma$ . These are found to be universal and their size can be calculated employing techniques from conformal field theory. For the Fortuin-Kasteleyn clusters relevant to the thermal phase transition we find agreement with these predictions from large-scale numerical simulations. For the spin clusters, on the other hand, the cluster numbers are not found to be consistent with the values obtained by analytic continuation, as conventionally assumed. We mention possible extension of the results for systems with quenched disorder, as well as for three-dimensional problems.

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- [2] I. A. Kovács, E. M. Elçi, M. Weigel and F. Iglói: Corner contribution to cluster numbers in the Potts models, Phys. Rev. B **89**, 064421 (2014), arXiv:1311.4186.
- [3] I. A. Kovács and F. Iglói: Corner contribution to percolation cluster numbers in three dimensions, preprint arXiv:1402.6535.



## C10 – Non-standard finite-size scaling at first-order phase transitions

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We note that the standard inverse system volume scaling for finite-size corrections at a first-order phase transition (i.e.,  $1/L^3$  for an  $L \times L \times L$  lattice in  $3D$ ) is transmuted to  $1/L^2$  scaling if there is an exponential low-temperature phase degeneracy. The goniuhedric Ising model which has a four-spin interaction, plaquette Hamiltonian provides an exemplar of just such a system. We use multicannonical simulations of this model to generate high-precision data which provides strong confirmation of the non-standard finite-size scaling law. The dual to the goniuhedric model, which is an anisotropically coupled Ashkin-Teller model, has a similar degeneracy and also displays the non-standard scaling.

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## C11 – Driven Heisenberg spin chain with arbitrary boundary twisting angle: Exact results

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We consider an open Heisenberg quantum spin chain, coupled at the ends to boundary reservoirs polarized in different directions, which sets up a twisting gradient across the chain. We demonstrate that the exact nonequilibrium steady state of the chain driven by boundary Lindblad operators can be constructed explicitly with a matrix product ansatz where the matrices satisfy the quantum algebra

$U_q[SU(2)]$ . Using this matrix product ansatz in the isotropic case, we calculate explicitly the magnetization profiles and magnetization currents.

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## **C12 – The critical Casimir force in a magnetic system: an experimental protocol**

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Close to a critical point of a continuous phase transition in a confined system fluctuations give rise to the critical Casimir force when the correlation length becomes of the order of the system size. Indirect measurements in  $^4\text{He}$  wetting films near the superfluid transition and both direct and indirect measurements in binary liquid mixtures have been performed. The Casimir force being a critical finite size effect, its universal functional form has been studied theoretically and numerically in the Ising and XY models as a generalized thermodynamic force,  $d\Omega/dL$ , where  $\Omega$  is the magnetic free energy. However, no measurement of the critical Casimir effect in magnetic systems has been performed. We introduce a new numerical experiment that follows a magnetic protocol which could in principle be adapted to experiments on thin film magnets.

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## C13 – Ageing of the 2+1 dimensional Kardar-Parisi-Zhang model

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Extended dynamical simulations have been performed on a 2+1 dimensional driven dimer lattice gas model to estimate ageing properties. The auto-correlation and the auto-response functions are determined and the corresponding scaling exponents are tabulated. Since this model can be mapped onto the 2+1 dimensional Kardar Parisi-Zhang surface growth [1, 2], our results contribute to the understanding of the universality class of that basic system. The violation of the fluctuation-dissipation relation is confirmed numerically [3]. I show comparison of results obtained on GPU-s CPU-s as well as on other models belonging to this universality class.

[1] G. Ódor, J. Kelling, Phys. Rev. E 84 (2011) 061150,

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## C14 – Entanglement spectra of interacting fermions in quantum Monte Carlo simulations

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In a recent article [1] T. Grover introduced a simple method to compute Renyi entanglement entropies in the realm of the auxiliary field quantum Monte Carlo algorithm. Here, we further develop this approach and provide a stabilization scheme to compute higher order Renyi entropies and an extension to access the entanglement spectrum. The method is tested on systems of correlated topological insulators.

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[2] F. F. Assaad, T. C. Lang, F. Parisen Toldin, arXiv:1311.5851.

## C15 – Planes, trains and polymers — the statistical physics of routing

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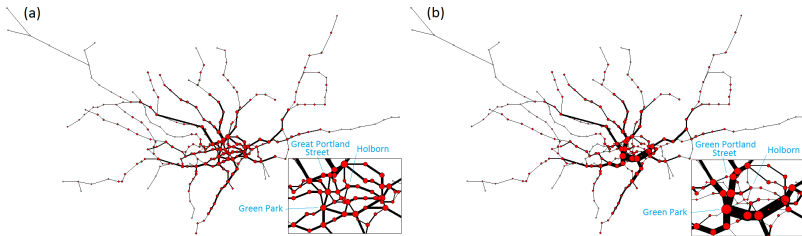
Optimizing paths on networks is crucial for many applications, from subway traffic to Internet communication. As global path optimization that takes account of all path-choices simultaneously is computationally hard, most existing routing algorithms optimise paths individually, thus providing sub-optimal solutions.

This work includes two different aspects of routing. In the first we employ the cavity approach to study analytically routing on a graph of given topology to predefined network routers and devise the corresponding distributive optimization algorithm. In the second we employ the physics of interacting polymers and disordered systems (the replica method) to analyse macroscopic properties of generic path-optimization problems between arbitrarily selected communicating pairs; we also derive a simple, principled, generic and distributive routing algorithm capable of considering simultaneously all individual path choices.

Two types of nonlinear interactions are considered with different objectives: 1) alleviate traffic congestion at both cyber and real space and provide better route planning; and 2) save resources by powering down non-essential and redundant routers/stations at minimal cost. This saves energy and man-power, and alleviates the need for investment in infrastructure. We show that routing becomes more difficult as the number of communicating nodes increases and exhibits interesting physical phenomena such as ergodicity breaking. The ground state of such systems reveals non-monotonic complex behaviours in average path-length and algorithmic convergence, depending on the network topology, and densities of communicating nodes and routers.

We demonstrate the efficacy of the new algorithm by applying it to: (i) random graphs resembling Internet overlay networks; (ii) travel on the London underground network based on Oyster-card data; and (iii) the global airport network. Analytically derived macroscopic properties give rise to insightful new routing phenomena, including phase transitions and scaling laws, which facilitate better understanding of the appropriate operational regimes and their limitations that are difficult to obtain otherwise.

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- [2] C. H. Yeung, D. Saad and K. Y. M. Wong, "From the Physics of Interacting Polymers to Optimizing Routes on the London Underground", *Proceedings of the National Academy of Sciences*, **110**, 13717-13722, (2013).



London underground traffic optimised to (a) minimise congestion and (b) consolidate routes and reduce the number active stations.

## C16 – Quantum environment for longer coherence time

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Decoherence is one of the main obstacles placed in the way of the correct functioning of quantum devices. It is an ubiquitous phenomenon, due to the unavoidable interaction between a quantum principal system and its environment, which becomes particularly disruptive when quantum properties are to be exploited and controlled. Despite being an ordinary effect, decoherence is not easily describable in a general framework, as it depends on several details of the physical setup. However, it has at least two key features: *i*) it is a dynamical process and *ii*) it is due to the interaction with an environment, which set the topic into the domain of the open quantum systems (OQS) dynamics. In this work, we make use of a recently proposed method[1] for studying the dynamical evolution of a generic quantum system subject to decoherence. From such treatment, an analytical expression for a consistent measure of the coherence time,  $\tau_d$ , emerges, and formally shows how, and why, decoherence depends on the number of dynamical variables of the environment. Based on this result we propose a strategy for extending  $\tau_d$ ; such strategy is finally implemented in two exemplifying situations where decoherence must be kept under control.

- [1] D.Calvani, A.Cuccoli, N.Gidopoulos, and P.Verrucchi, PNAS **110** (2013) 6748.

## C17 – Non-Ising critical point in a fluid with short-ranged interactions

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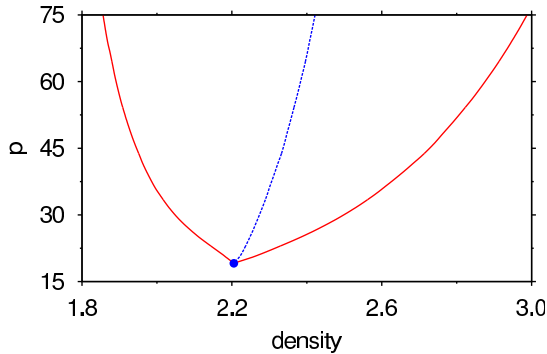
It is commonly accepted that fluids undergoing a liquid-vapor type transition belong to the universality class of the Ising model. In the context of finite-size scaling, this means that the density difference between the two phases at the critical point vanishes  $\propto L^{-x}$ , where  $L$  is the linear size of the system (simulation box) and  $x = 1/8$  for the two-dimensional (2D) Ising model. Here, I present a counter example, where instead  $x \sim 0.5$  is observed. For the susceptibility, a scaling  $\propto L^y$  is found,  $y \sim 1$ , consistent with 2D hyperscaling  $2x + y = 2$ .

The fluid is a 2D system of  $N$  point particles, interacting via a pair potential  $V = \sum_{i < j} u_{ij}$  that is strictly short-ranged,  $u_{ij} = \epsilon(1 - |\vec{d}_i \cdot \vec{d}_j|^p)H(a - r_{ij})$ , with  $r_{ij}$  the distance between particles  $i$  and  $j$ , interaction range  $a$ ,  $H(x)$  the Heaviside unit step function,  $\epsilon$  a coupling constant to set the temperature scale, and  $\vec{d}_i$  a 2D unit vector denoting, say, the orientation of particle  $i$ . Provided the exponent  $p$  is large enough, this system undergoes a first-order phase transition between a high density liquid phase, and a low density vapor [1]. By lowering the exponent  $p$ , this first-order transition terminates at a critical point, characterized by the above mentioned critical exponents  $x$  and  $y$ , which differ distinctly from 2D Ising values.

I will present the simulation analysis that was performed to reach these conclusions. A paramount ingredient of this analysis was a scheme to enable the extrapolation of simulation data obtained for one value of  $p$ , to different (nearby) values. Since  $p$  is not a field variable (i.e. it does not appear as a prefactor in the potential energy) one cannot use the standard histogram reweighting algorithm of Ferrenberg and Swendsen [2] for this purpose.

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The binodal (coexistence curve) of our non-Ising model.

## C18 – Wave function engineering in quantum nanostructures

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Quantum structures (called sometimes artificial atoms) which can be steered from the outside are highly relevant to new technologies in which the control and manipulations of electron spin and wave functions play an important role. We have considered nanostructures composed of a semiconductor quantum dot surrounded by a quantum ring. The properties of such nanostructures can be strongly modified by changing the shape and the height of the confinement potential. The manipulation of these parameters by e.g. electrical gating leads to the change of the shape and the radial distribution of wave functions which strongly influence many properties.

We have shown that such wave function engineering can alter [1, 2]:

- a) the relaxation time of nanostructure used as a spin qubit or a memory device by orders of magnitude
- b) the cross-section for intraband infrared or microwave absorption from large to negligible
- c) the conducting properties of a single nanostructure and of an array of dotting nanostructures from highly conducting to insulating.



Thus the basic issues of quantum mechanics can be explored to optimize the specific properties of nanostructures by means of sophisticated design.

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## Poster Presentations

# P1 – The crystal field effects for the Ising bilayer system consisting of spin-1/2 and spin-3/2

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The study of magnetic thin films consisting of various magnetic layered structures or superlattices has recently received intense attention for both theoretical and experimental objectives [1]. These materials are made up of multiple layers of different magnetic substances, thus there is a high potential for technological advances in information storage and retrieval and in synthesis of new magnets for a variety of applications and they also present some interesting novel magnetic properties such as giant magnetoresistance [2], surface magnetic anisotropy [3], enhanced surface magnetic moment [4] and surface magnetoelastic coupling [5].

In this study, a model consisting of two Bethe lattices each with a branching ratio of  $q$  Ising spins with one layer having spin-3/2 with nearest-neighbor (NN) interaction  $J_1$  and crystal field interaction  $D$ , and the other having spin-1/2 with NN interaction  $J_2$  is considered. The layer with spin-3/2 is laid over the top of the other with spin-1/2 and the two layers are tied together via an interaction between the vertically aligned spins denoted as  $J_3$ . The variations of the order-parameters and the free energy are investigated using the exact recursion relations in a pairwise approach to obtain the temperature dependent phase diagrams of the model by considering only the ferromagnetic ordering of the layers, i.e.  $J_1 > 0$  and  $J_2 > 0$ , and ferromagnetic or antiferromagnetic ordering of the adjacent NN spins of the layers,  $J_3 > 0$  or  $J_3 < 0$ , respectively. Besides the second-order phase transition lines with different kinds of behaviors, the first-order phase transition lines either ending at a tricritical point or at an isolated critical point are found. The model presents compensation temperatures when  $J_2$  of the lower layer can compete with  $J_1$  of the upper layer. The paramagnetic phase is also divided into two phases by studying the thermal behaviors of the quadrupolar moment for the

layer with spin-3/2.

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## **P2 – Partition function of the monomer-dimer model**

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In this poster, I will discuss the generalized monomer-dimer model and show how Grassmann variables can be used to express the partition function, and compute correlation functions exactly.

- [1] Poster partially based on <http://arxiv.org/pdf/1402.5512.pdf>.

## P3 – Crystallization mechanism in melts of short n-alkane chains

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Despite the long-standing research interest in crystallization in polymer melts, many fundamental aspects of the crystal nucleation and growth mechanisms are still subject of discussion [1]. In the traditional picture of the early stages of the polymer crystallization, the Bragg peaks are observed after the induction period in wide angle X-ray scattering (WAXS). But in 1990's small angle X-ray scattering (SAXS) peaks were reported in many experiments during induction period [2, 3]. These SAXS peaks were claimed to be due to the presence of ordered melt before occurrence of nucleation event. Theories have been proposed to explain these SAXS peak [4, 5]. Given the high degree of complexity that long polymer chains pose, a basic comprehension of how even relatively short chains crystallize is of fundamental importance in order to build a coherent theory. Crystal nucleation in alkanes has been addressed in several computer simulation studies in the 90s [6, 7, 8] and a scenario for the nucleation mechanism has been suggested. Due to the limited computer resources available at the time, however, these works were based on one simulation trajectory each (except Ref. [6]). Considering the limited amount of data available in the literature on the nucleation and growth mechanism in short chain alkanes, we identify the microscopic mechanisms of homogeneous crystal nucleation and growth. For the nucleation process, we observe that chains first align and then straighten. Then the local density increases and finally the monomer units become ordered positionally. The subsequent crystal growth process is characterized by a sliding-in motion of the chains. This process is cooperative, i.e. neighboring chains tend to get attached in clusters rather than independently.

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## P4 – Irreversibility by competition for a Glauber-Ising model by means of the entropy production

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An irreversible and out of equilibrium system is analyzed by means of a stochastic dynamics based on an approach that aims to understand the macroscopic effects as a consequence of the microscopic characteristics. The study focus on the kinetic phase transitions that take place by assuming a lattice model, intended to describe the stationary states by the entropy production, which characterize the system behavior, clarifying the reversibility conditions. Thus a kinetic Ising model with up-down symmetry and under the influence of two competing Glauber dynamics is analyzed. In this sense one considers a square lattice formed by two sublattices interconnected, which are in contact with two heat baths at different temperatures. The study is made by means of the analytical approach of a mean-field approximation and Monte Carlo simulations. The results show a phase transition of the second order in the steady state regime, which is evidenced by a logarithmic divergence of the entropy production derivative.

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## P5 – MuCa vs WL: A tight race

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We perform a competitive analysis to study the relative performance of the two best-known generalized-ensemble algorithms: the multicanonical Monte Carlo and the Wang-Landau method. To keep things as simple and clear as possible, we take the exactly solvable two-dimensional Ising model as test case and we show also some results for the three dimensional Ising model.

## P6 – Current fluctuations in a temporally correlated zero-range process

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We study, both analytically and numerically, an open boundary version of the on-off zero range process (ZRP) introduced in [1]. In this model the departure rates from a node depend not only on its occupation number, but also on previous arrivals. This condition mimics the instantaneous congestion of customers also observed in human dynamics, where the temporal correlations are not negligible.

We focus on the large deviations of current in this model. Analytical calculations for a one-site system show that, although the steady state corresponds to that of a Markovian ZRP with modified hopping rates, the probability of rare currents differs significantly from the Markovian case. In particular, we find evidence for a novel memory-induced dynamical phase transition. The analytical results are tested against Monte Carlo simulations and an advanced numerical method which has been developed to evaluate large deviation functions directly [2].

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## P7 – PageRank model of opinion formation on Ulam networks

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The understanding of mechanisms of opinion formation in the modern society is at the heart of a newly emerged research field, known as sociophysics [1]. Among a large number of voter models, developed during last few decades, we consider the PageRank model of opinion formation on Ulam networks [2]. The latter networks, generated by the intermittency map and the typical Chirikov map, share certain similarities with such scale-free networks as, e.g., the World Wide Web (WWW) [3]. On the other hand, the PageRank model of opinion formation introduces the notion of importance of a node, naturally reproducing the real society, where each person has its degree of authority [4]. In the present work we show that the opinion formation process on Ulam networks have certain similarities, but also distinct features compared to the WWW. We attribute these distinctions to internal differences in network structure of the Ulam and WWW networks. Additionally, we study the influence of network elite on opinion formation process and consider the Sznajd model [5], generalized for scale-free networks, which protects opinion of small communities.

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## **P8 – Non-equilibrium steady states of Fokker-Planck-Boltzmann equation**

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In the presence of forcing and dissipation, widely separated in scale, the Boltzmann equation is known to display non-equilibrium steady states where energy and mass is transported conservatively. We consider an approximation to the Boltzmann equation with the same quadratic non-linearity that exhibits such types of solutions, and provide numerical and analytical predictions for the relation between the forcing and dissipation scales and the thermodynamic quantities of the system. We compare our results with a differential approximation model, which has been used previously to derive predictions.

## **P9 – Condensation of large fluctuations in a thermodynamical system**

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Condensation of fluctuations is an interesting phenomenon conceptually distinct from condensation on average. One striking feature is that, contrary to what happens on average, condensation of fluctuations may occur even in the absence of interactions or external constraints. This surprising phenomenon is investigated, in and out of equilibrium, in the context of simple models of classical statistical mechanics, like the Gaussian model or the Spherical model, chosen as paradigmatic non-interacting or interacting systems. The explanation emerges from the duality between large deviation events in the given system and typical events in a new and appropriately biased system. It is shown that the bias in the companion system induces a mean-field-like effective interaction. Phase diagrams, covering both the equilibrium and the off-equilibrium regimes, are derived for observables representative of generic behaviors. The difference in the experimental protocols required to observe the two facets of condensation is highlighted.

## P10 – The Navajo and Quiche myths: a comparative study on the mythology of Amerindians

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The theme of my talk is to discuss a new approach to comparative mythology which involves the use of network theory. By studying the social networks of classical texts and comparing them to social networks of “real life”, the aim of this approach is to be able to say something about their historicity, among other things. This idea was first put forward [1] and the present work is part of an ongoing cooperation whose aim is to extend this innovative approach to different cultures [2] as well as deepen the analysis of texts using network theory.

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## P11 – Evolved model regulatory networks form meta-networks in genotype and phenotype space

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A model population of Boolean networks evolved under selection for short dynamical attractors, form a meta-network in genotype space whose nodes are Boolean networks which are connected by an edge if they are one mutation away from each

other. Co-evolved networks are closer to each other in genotype space compared to the randomized networks, in the sense that the average mutational distance between the evolved networks is smaller than those of randomized networks. The degree distributions of the meta-networks formed in genotype space generally fit Poisson distributions with the same mean value for independently evolved populations. Most of these meta-networks have connected components containing more than half of the networks within the population. The randomized counterparts of the evolved networks, however, do not have any neighbors in the genotype space, since the minimum mutational distance between the randomized networks is larger than one. The Boolean networks form a meta-network also in phenotype space, where two Boolean networks are connected by an edge, if they share at least one attractor. The edges are weighted by the sizes of the basins of attraction of the shared attractors and different threshold values are used to eliminate weak connections. The meta-networks in the phenotype space of the evolved populations exhibit degree distributions which increase with the degree and the sizes of their largest connected components decrease slower with the increasing threshold compared to the meta-networks of the randomized populations, suggesting a percolation threshold which goes to zero with the system size.

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## P12 – Dynamic phase transitions in a cylindrical Ising nanowire

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Magnetic nanowire systems have attracted considerable attention not only because of their academic interest, but also their technological applications. In particular, in the areas of magnetic recording media, spin electronics, optics, sensors and thermoelectronics devices [1]. It has been also reported that Ni nanowires can be used in bioseparation and have higher yields compared with magnetic polymer microspheres [2]; hence this provides a new chance for magnetic nanowires to be applied in biomedical fields. In the experimental area, the magnetic nanowires have been synthesized and their magnetic properties have been investigated, such as Fe-Co, Co-Pt, Ni,  $\text{Ga}_{1-x}\text{Cu}_x\text{N}$ , Fe,  $\text{Fe}_3\text{O}_4$ , Co, Fe-Pt, Ni-Fe, Co-Cu etc [3].

While the equilibrium properties of the magnetic nanowires have been investigated within the several theoretical methods in equilibrium statistical physics, as far as we know, the dynamical aspects of the magnetic nanowires have not been investigated. The purpose of the paper is to calculate and characterize the nature (first- or second-order) of dynamic phase transitions (DPTs) in a cylindrical Ising nanowire system under a time-dependent oscillating external magnetic field for both ferromagnetic and antiferromagnetic interactions by employing the EFT with correlations and the Glauber-type stochastic dynamics. Temperature dependence of the dynamic magnetizations, the dynamic total magnetization, the hysteresis loop areas and the dynamic correlations are investigated in order to characterize the dynamic phase transition temperatures and the compensation behaviors. The system strongly affected by the surface situations. Some characteristic phenomena are found depending on the ratio of the physical parameters in the surface shell and the core. According to the values of Hamiltonian parameters, five different types of compensation behaviors in the Neel classification nomenclature exist in the system. The system also exhibits a reentrant behavior.

This work was supported by Nevsehir Hacı Bektas Veli University Research Funds, Grant no. 2012/12.

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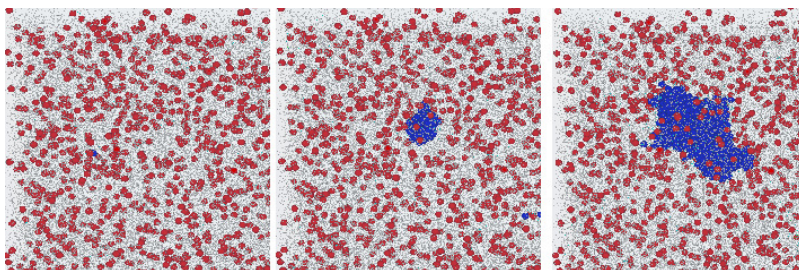
## P13 – Influence of random pinning on the crystallization process in suspensions of hard spheres

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We discuss crystal formation in supersaturated suspensions of monodisperse hard spheres with a concentration of hard spheres randomly pinned in space and time. The pinning procedure introduces an external length scale and an external time scale that restrict the accessible number of configurations and ultimately the number of pathways leading to crystallization. We observe a significant drop in the nucleation rate density at a characteristic pinning concentration that can be directly related to the structure of the critical nucleus and the dynamics of its formation in the unpinned system.

[1] Sven Dorosz and Tanja Schilling, JCPT, Vol.4 No.2, Jan 2014



A series of snapshots of a typical nucleation event (blue) out of an overcompressed fluid (grey) in the presence of randomly pinned hard spheres (red).

## P14 – Fragmentation of Potts clusters

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The random cluster model is at the heart of a range of models in statistical physics, including uniform spanning trees, percolation and the Potts model. Many geometric and fractal aspects have been analysed, in particular at criticality, and a related zoo of exponents is known exactly or at least accessible by numerical methods. The fragmentation of clusters is a process of general importance for the modeling of a wide range of phenomena, including polymer fragmentation and processes in porous media. We use extensive numerical simulations employing a recent efficient implementation of Sweeny's single-bond algorithm to study the distribution of cluster sizes as well as the density of fragmenting (or bridge) bonds relevant to the fragmentation properties. The latter quantity is of additional importance for algorithmic aspects such as the observed critical speeding up of the single-bond dynamics.

## P15 – Deconfinement and topological-sector fluctuations at the Berezinskii-Kosterlitz-Thouless phase transition

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We investigate the emergent electromagnetism of the 2dHXY model [1] at finite temperature. We find the model to be governed by laws entirely analogous to Maxwell's equations. We show that two-dimensional Maggs-Rossetto protocol [2] extended to the Grand Canonical Ensemble is equivalent to the 2dHXY model. This mapping clearly illustrates the topological nature of the Berezinskii-Kosterlitz-Thouless phase transition [3]: the deconfinement of the emergent charge

above the phase transition leads to topological-sector fluctuations in the emergent electric field; this is characterized by an order parameter calculated via the winding number of the system.

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## P16 – Hyperscaling above the upper critical dimension in Ising models with long range interactions

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It is well known that standard hyperscaling ( $\nu d = 2 - \alpha$ ) and universal finite-size scaling break down above the upper critical dimension  $d = d_c$ , where critical exponents take on their Landau values. This is due to dangerous irrelevant variables in the renormalization group formalism. A recently developed theory ascribes the breakdown of hyperscaling to a separation of the correlation length scale  $\xi_L$  from the underlying system length scale  $L$ , and introduces a new critical exponent via  $\xi_L \sim L^q$ . While  $q = 1$  for  $d \leq d_c$ ,  $q = d/d_c$  above the upper critical dimension. Taking proper account of these different length scales allows one to extend hyperscaling to all dimensions via  $\nu d/q = 2 - \alpha$ . It also modifies finite scaling in such a way that, e.g., the standard form for the susceptibility  $\chi_L \sim L^{\gamma/\nu}$  becomes  $\chi_L \sim L^{q\gamma/\nu}$ .

Here we consider an Ising model with long-range interaction strength decaying as  $1/r^{d+\sigma}$ , for which  $d_c = 2\sigma$ . In particular, we simulate the system in  $d = 1$  dimension with periodic boundary conditions. The simulation was implemented using a

cluster Monte Carlo method for spin systems with long-range interaction [3], which is based on the Swendsen-Wang cluster algorithm through Fortuin-Kasteleyn spin representation. Implementing the simulations for a number of different values of  $\sigma$ , we verify the new scaling form for the correlation length and the modified form for finite-size scaling and verify that the new critical exponent is  $q = d/d_c = 1/2\sigma$ .

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## **P17 – Structure optimization of BLN protein models combining local-search, evolutionary, and genetic approaches**

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Establishing relations between the amino acid sequence of a protein and its spatial structure is a very important and challenging task. When analysing the forces affecting the protein folding, the investigation of the related free energy landscape is of central importance. Thereby, to obtain the ground state and low-energy metastable states, highly efficient structure optimization tools are needed.

Here, we study the properties of genetic local-search type optimization approaches, in particular of thermal cycling (TC) [1] and systematic-crossover local-search (SCLS) algorithms. For this aim, we focus on the BLN protein model, designed by J.D. Honeycutt and D. Thirumalai [2]. We consider 46-, 58-, and 69-bead sequences from Refs. [2, 3]; the 69-bead sequence seems to be the largest BLN model treated in the literature up to now.

In all these cases, the TC and SCLS algorithms reliably find the global minimum within reasonable computing times. Both algorithms proved to be far more efficient than multi-start local-search and simulated annealing approaches.

In the present work, to the best of our knowledge, the BLN model with rigid bond lengths is studied in detail for the first time. We compare our results to



the properties of the extended model by Berry et al. [4], in which stiff spring-like bonds are substituted for the rigid bonds: The hardening of the spring constants causes several level crossings of the metastable states. For the 46-bead model, this concerns even the ground state.

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## P18 – Nonequilibrium processes in the vicinity of hydrodynamic states

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The Chapman–Enskog method is generalized on the basis of the Bogolyubov idea of the functional hypothesis (see, for example, [1]). A theory that describes a nonequilibrium state of a gas by the usual hydrodynamic variables  $\zeta_\mu(x, t)$  and arbitrary additional local variables  $\theta_i(x, t)$  has been constructed. The gradients of all these parameters and the deviations  $\delta\theta_i(x, t)$  of the variables  $\theta_i(x, t)$  from their hydrodynamic values  $\theta_i(x, \zeta(t))$  are assumed to be small and are estimated by two independent small parameters  $g, \lambda$ . The proposed theory is nonlinear in the variables  $\delta\theta_i(x, t)$  too.

The usual Chapman–Enskog method leads to the solution of Fredholm integral equations of the first kind with an operator  $\hat{K}$  given by the linearized collision integral. The proposed theory leads to the solution of linear integral equations of a more complicated nature with the same operator  $\hat{K}$ . Some of them are eigenvalue problems for the operator  $\hat{K}$  and describe the kinetic modes of the system.

The proposed theory is applied to the solution of a modified Grad problem. Grad formulated his problem in his 13-moment approximation for the solution of kinetic equations [2]. In his theory nonequilibrium states of a gas are described, in

addition to the usual hydrodynamic variables, by the fluxes of energy  $q_n(x, t)$  and traceless momentum  $\pi_{ln}(x, t)$ . In fact, these fluxes are considered as small quantities of the same order  $\lambda$  and the Grad distribution function includes only terms of the orders  $g^0\lambda^0$ ,  $g^0\lambda^1$ . Moreover, it corresponds to the one-polynomial approximation in the Burnett method and his method is based on a very approximate solution of the eigenvalue problem for the operator  $\hat{K}$ . In our modification of the Grad problem, a nonequilibrium state of a gas is described by the usual hydrodynamic variables and small deviations  $\delta q_n(x, t)$ ,  $\delta \pi_{ln}(x, t)$  of the above-mentioned fluxes from their hydrodynamic values  $q_n(x, \zeta(t))$ ,  $\pi_{ln}(x, \zeta(t))$ . In the simplest approximation this leads to a theory of the Maxwell relaxation. The Bogolyubov reduced description method, based on his idea of the functional hypothesis, gives an adequate solution of the problem.

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## P19 – Dynamics of spherical model with correlated noise

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The dynamics of a (mean) spherical model with correlated noise is investigated. The noise possesses a fractional brownian motion with Hurst index  $H$ , and the analysis is based on exact results obtained for the two-time autocorrelation and response function. The behaviour of the system is compared to the work of Godrèche-Luck[1], where the noise is uncorrelated. Not only the dynamics of the present case is richer (due to the extra parameter  $H$ ), but displays a non-trivial interplay between the dissipative part and noise term.

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## **P20 – Ground-state, magnetic and partition function zeros properties of the spin-1 Ising-Heisenberg model on a diamond chain**

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We study the ground state, magnetic and partition function zeroes properties of the spin-1 Ising-Heisenberg model on a diamond chain using the transfer matrix method. The model demonstrate a large variety of ground-state phases. The existence of the magnetization plateaus have been observed at one third as well as two third of the saturation magnetization. The Yang-Lee and Fisher zeros distributions are studied numerically for a variety of value of model parameters. The existence of the usual  $\sigma = -\frac{1}{2}$  and unusual  $\sigma = -\frac{2}{3}$  Yang-Lee edge singularity exponents are shown.

## **P21 – Modelling of topological defects entangled around nanoparticles of nematic liquid crystal colloids**

**Anja Humpert**

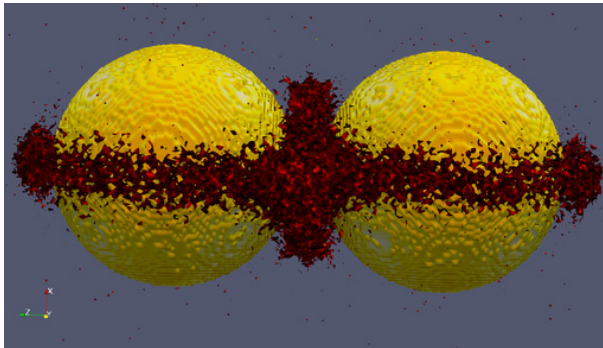
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We aim to study topological defects around nanoparticles in liquid crystals. Large-scale molecular dynamics simulations are used to obtain a better understanding of

their molecular-level behaviour. The main focus is to study the defect structures around nanoparticles inserted into a nematic as a function of particle separation and to measure the free-energy associated with such arrangements. Spherical nanoparticles of different sizes inserted into a nematic were simulated using the Gay-Berne (GB) potential [1]. Around the nanoparticles the liquid crystal molecules are frustrated. This is due to the competition between aligning along the main direction of the liquid crystal molecules, called the director, and the anchoring conditions at the nanoparticles' surface. For homeotropic, normal, anchoring, Saturn ring defects were found [2], while for planar anchoring, Boojum defects were observed, which is in excellent agreement with Laundau-de Gennes theory (LdG) [3]. For larger colloids with homeotropic anchoring, in experiments the Satellite defect was observed to be stable [4]. This defect has a dipolar structure in the director field, whereas the Saturn ring defect has a quadrupolar structure. By initially applying an external field, this defect structure can also be observed for small nanoparticles. We have also carried out molecular simulations of pairs of colloids approaching each other. At small particle separations the defect loops around each colloid start to bend and at very close distances entangled defect structures were observed [5].

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Entangled defect structure

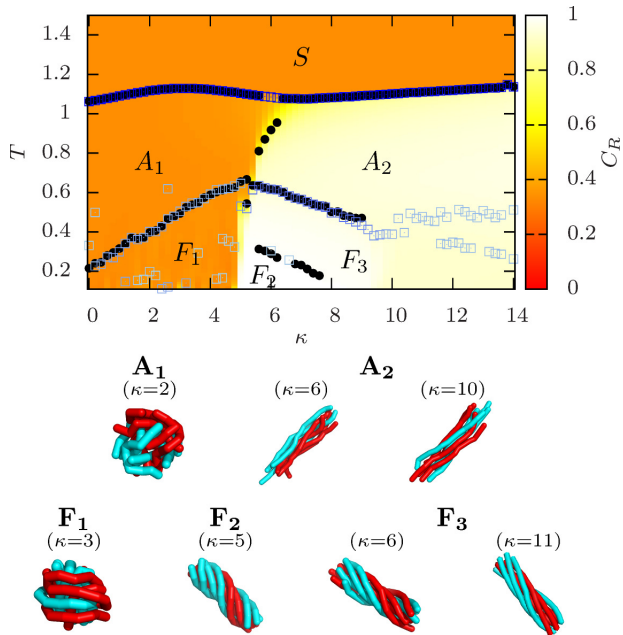
## **P22 – From amorphous aggregates to polymer bundles: The role of stiffness on structural phases in polymer aggregation**

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We study the aggregation transition of a finite polymer system in dependence on the bending stiffness  $\kappa$  with the help of parallel multicanonical simulations. In order to distinguish amorphous aggregates from polymer bundles we introduce an order parameter, measuring the correlation of the end-to-end vectors. With the help of this order parameter, we construct full  $T$ - $\kappa$  phase diagrams for systems with 2 and 8 polymers and discuss the occurring phases from amorphous aggregates to bundle structures. For an intermediate stiffness range we find multiple aggregated phases which change with increasing number of polymers and discuss their nature with the help of microcanonical analyses. We show that the stiffness of semiflexible polymers plays a key role in whether the system forms amorphous aggregates or bundle structures [1].

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Phase diagram for 8 polymers consisting of  $N = 13$  monomers each, combining the surface plot of the end-to-end correlation parameter, the maxima of the heat capacity (black dots) and the temperature derivative of a phase separation parameter (blue squares). We identify several structural phases, namely  $S$  (separated),  $A_i$  (aggregated) and  $F_i$  (“frozen”), and present typical conformations for the low-temperature phases.

## **P23 – Adsorption of a simple fluid in a nanopore: influence of system and reservoir size on the intermediate states visited**

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Adsorption of fluids in a nanoporous solid is of great importance regarding porous materials characterization, catalysis, environment, energy . . . Besides experimental investigations, molecular simulation or density functional theory calculations provide valuable information for experimental data analysis, and possibly predictions. We focus on the adsorption properties of a fluid confined in simple pore geometries (cylindrical and slit pore) in equilibrium with a reservoir. We investigate the effect of system and reservoir size. The system generally exhibits hysteresis in the adsorption and desorption isotherms, hindering the determination of equilibrium states. It is shown that, even for small system or reservoir size, the isotherms still exhibit discontinuities associated with inhomogeneous states that break the pore symmetry. We examine the physical relevance of these intermediate states for the liquid/vapour transition of confined fluid, and explore the validity of thermodynamic integration for free energy calculations, which are required for the determination of the coexistence and possibly the energy barriers associated with the transition.

## P24 – Distribution of dynamical quantities in the contact process, random walks, and quantum spin chains in random environments

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We study the distribution of dynamical quantities in various one-dimensional, disordered models the critical behavior of which is described by an infinite randomness fixed point. In the *disordered contact process*, the survival probability  $\mathcal{P}(t)$  is found to show multi-scaling in the critical point, meaning that  $\mathcal{P}(t) = t^{-\delta}$ , where the (environment and time-dependent) exponent  $\delta$  has a universal limit distribution when  $t \rightarrow \infty$ . The limit distribution is determined by the strong disorder renormalization group method analytically in the end point of a semi-infinite lattice, where it is found to be exponential, while, in the infinite system, conjectures on its limiting behaviors for small and large  $\delta$ , which are based on numerical results, are formulated. By the same method, the survival probability in the problem of *random walks in random environments* is also shown to exhibit multi-scaling with an exponential limit distribution. In addition to this, the (imaginary-time) spin-spin autocorrelation function of the *random transverse-field Ising chain* is found to have a form similar to that of survival probability of the contact process at the level of the renormalization approach. Consequently, a relationship between the corresponding limit distributions in the two problems can be established. Finally, the distribution of the spontaneous magnetization in this model is also discussed.

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## P25 – Cluster size distribution in the autocatalytic growth model

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Colloid formation, as well as polymerization processes of various kind, usually involve chemical reactions. Such phenomena may be described theoretically by so called reaction-aggregation equations. We present a particular reaction-aggregation model, where in the absence of coagulation, analytical solution can be obtained for arbitrary values of the model parameters. This result is of a practical importance, because coagulation may be experimentally switched off quite easily. If this is the case, the present model may provide good description of the real experimental situation.

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## P26 – On the uniform sampling of ground states in the 2D $\pm J$ Ising spin glass model

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It is well known that the Edwards-Anderson Ising spin glass with discrete coupling distribution results in an extensive ground-state degeneracy. As the number of ground states hence grows exponentially with system size  $L$ , an exact enumeration is not practical, except for very small systems. This even applies to the otherwise well tractable model in two dimensions. There, exact ground states can be generated in polynomial time using one of several known mappings to minimum-weight perfect matching problems. While the resulting algorithm can be modified to generate random ground states in the presence of degeneracies, these are not in general produced with uniform probabilities. Here, we introduce an approach that achieves approximate uniform sampling. The algorithm is based on a cluster analysis of connected domains of free spins resulting from inputs generated by the matching approach which are then used as state space for a suitably adapted Markov chain sampling.

## P27 – Corner contribution to percolation cluster numbers in three dimensions

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In three-dimensional critical percolation we study numerically the number of clusters,  $N_\Gamma$ , which intersect a given subset of bonds,  $\Gamma$ . If  $\Gamma$  represents the interface between a subsystem and the environment, then  $N_\Gamma$  is related to the entanglement entropy of the critical diluted quantum Ising model. Due to corners in  $\Gamma$  there are singular corrections to  $N_\Gamma$ , which scale as  $b_\Gamma \ln L_\Gamma$ ,  $L_\Gamma$  being the linear size of  $\Gamma$  and the prefactor,  $b_\Gamma$ , is found to be universal. This result indicates that logarithmic

finite-size corrections exist in the free-energy of three-dimensional critical systems.

## P28 – Lee-Yang-Fisher zeros for the Ising model on complex networks

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We analyze the partition function of the Ising model on graphs of two different types: (i) a complete graph, when all graph nodes are mutually linked and (ii) an annealed scale-free network with the node-degree distribution decaying  $P(k) \sim k^{-\lambda}$ . We are interested in zeros of the partition function  $Z$  in the case of complex temperature  $t$  or external field  $h$  (Fisher and Lee-Yang zeros correspondingly) [1, 2]. The study of partition function zeros gives quantitative information about phase transitions occurring in the system. In particular, for the second order phase transition, location and motion of the zeros allows to calculate the critical temperature, critical exponents  $\alpha$ ,  $\beta$ ,  $\delta$  and the critical amplitude ratio  $A_+/A_-$ .

By the present study, we accomplish the Lee-Yang [3] and Fisher [4] zeros analysis for the Ising model on a complete graph. For the model on an annealed scale-free network, we find an appropriate integral representation for the partition function. In particular, for  $h = 0$  it reads:

$$Z \sim \int_0^{+\infty} e^{-tu^2 - u^4} du, \quad \lambda > 5, \quad (1)$$

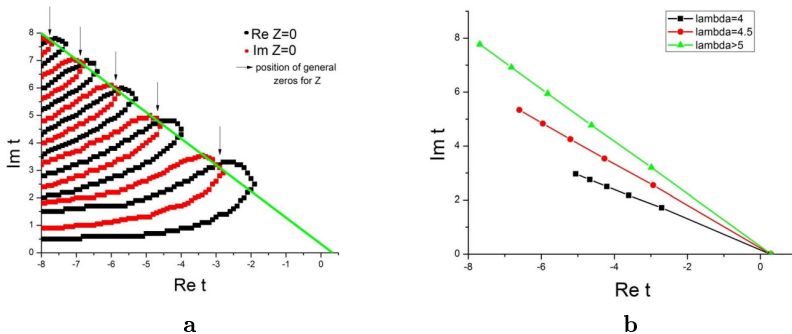
$$Z \sim \int_0^{+\infty} e^{-tu^2 - u^{\lambda-1}} du, \quad 3 < \lambda < 5. \quad (2)$$

Here,  $t$  is appropriately normalized temperature variable.

One of the obtained results is demonstrated by Fig. a, where the solutions of the equations  $\text{Re} Z = 0$  and  $\text{Im} Z = 0$  with  $Z$  given by Eq. (1) are shown by dark and light curves correspondingly (black and red online). Crossings of these curves form the line of Fisher zeros. In the vicinity of the critical point,

this line makes an angle  $\varphi$  with the real part of the complex temperature plane. Note, that the case  $\lambda > 5$  reproduces behaviour of zeros for the Ising model on a complete graph. For  $3 \leq \lambda < 5$  the angle  $\varphi$  appears to be  $\lambda$ -dependent (see Fig. b). In turn, this gives access to the ( $\lambda$ -dependent) values of the critical exponents and critical amplitudes ratios of the Ising model on the scale-free network.

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## P29 – A simple mechanism for controlling oscillations in coupled genetic circuits

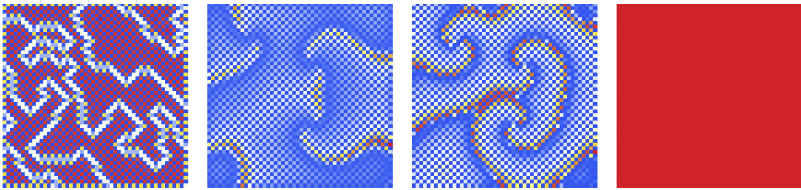
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We study a system of coupled genetic circuits, so-called bistable frustrated units. Individual units show excitable or oscillatory behaviour depending on the choice of parameters [1]. The same regimes are observed also for coupled units when a single uniformly chosen bifurcation parameter is varied. By monotonically tuning this parameter we can generate pattern formation over a finite time interval and control the duration of oscillations. Depending on the tuning speed, the network

topology and the coupling strength, we observe a rich dynamics with different time scales, self-organized pacemakers, spiral patterns, and planar waves. To demonstrate the complexity of the dynamics, we perform a detailed bifurcation analysis for two coupled units and indicate how it extrapolates to a larger network.

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Formation of a spiral pattern on an undirected rectangular lattice

## P30 – Capillary wave and dynamical interfacial tension for a two-component Bose-Einstein condensate in strong segregation: I. Planar limit

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We employ Bogoliubov analysis to study capillary wave (ripples) at a planar interface of a two-component Bose-Einstein condensates in strong segregation analytically and numerically. We propose a set of ansatz functions for the order parameters with both spatial and phase fluctuation in the limit of a small oscillation in compressible superfluids. Incompressibility is recovered when the phase velocity of the surface wave is small compared to the sound wave of the condensates. Combining the far-field and near-field behavior of the Bogoliubov-de Gennes (BdG) equations for the condensates, we obtain approximated analytic solutions in long wavelength limit. With which and the peculiar boundary conditions, we solve BdG equations numerically by a successive over relaxation method. We then

study the energy associated with the presence of a capillary wave and use the analytical solutions for BdG equations to obtain dispersion relation and dynamic surface tension. This dispersion relation agrees with the prediction of classical incompressible fluids but with a correction linear to the wavenumber of the surface wave due to the highly compressible nature of the condensates.

## P31 – Statistical distributions and the entropy considerations in genetics

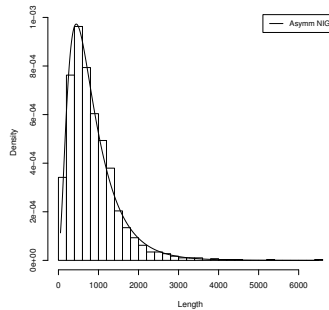
Krystyna Lukierska-Walasek<sup>1</sup>, Krzysztof Topolski<sup>2</sup>

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In last years appeared the possibility to provide some knowledge of genome sequence data in many organisms. The genome have been studied intensively by number of different method, for example [1]-[5]. In papers [3] and [4] the Zipf approach to analyzing linguistic texts has been extended to statistical study of DNA base pair sequences. A language is characterized by some alphabet with letters, which form words as sequence of  $n$  letters. Languages have very different alphabets: computers 0,1 (two bits), English language 27 letters with space and DNA four nitric bases: G(*guanine*), A(*adenine*), C(*cytosine*), T(*thymine*). Zipf's law implies the statistical distributions of hyperbolic type, which can describe the properties of stability and entropy loss in linguistics [6]. Similar situation can occur in a genome sequence data which carries the genetic information. We present the information theory from which follows that if the system is described by distributions of hyperbolic type it leads to the possibility of entropy loss. We try to find the correspondence between the histograms of gene lengths and the hyperbolic distributions for some bacteria, as *Borelia burgdorferi*, *Escherichia coli* and *Saccharomyces cerevisiae*. We model a gene length histograms using Generalized Inverse Gaussian hyperbolic distributions. Fig. 1 present histogram of the gene length in the genome of the *Borrelia burgdorferi* with the fit of the inverse Gaussian distribution. We present also the number of repetitions of genes in the genomes of *Escherichia coli* and *Borelia burgdorferi*. Distributions of repetitions of genes in genome are represented by distributions of hyperbolic type.

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Histogram of the gene length in the genome of the *Borrelia burgdorferi* with the fit of the inverse Gaussian distribution.

## P32 – Competing contact processes in the Watts–Strogatz network

**Marcin J. Rybak, Krzysztof Malarz, Krzysztof Kułakowski**

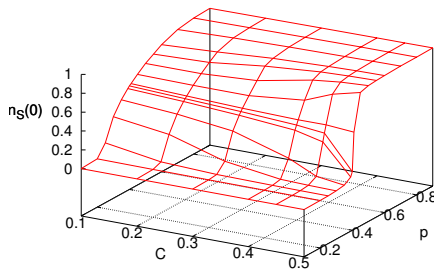
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Two competing processes [1, 2] are simulated on the Watts–Strogatz network [3]. The network's nodes are decorated with spin-like variables  $s_i \in \{S, D\}$ . During simulation each  $S$  node having a  $D$ -site in its neighbourhood converts this neighbour from  $D$  to  $S$  state. Conversely, a node in  $D$  state having at least one neighbour also in state  $D$ -state converts all nearest-neighbours of this pair into  $D$ -state [4]. The latter is realized with probability  $p$ . After long enough simulation

time  $T$  the system reaches a stationary state with all sites either in  $S$  or all sites in  $D$ -state.

We construct a surface of unstable fixed points in  $(\mathcal{C}, p, n_S(0))$  space, where  $\mathcal{C}$ ,  $p$ ,  $n_S(0)$  are the network clustering coefficient, the probability of  $D$ -like process and an initial fraction of nodes in  $S$  state. For points on this surface half of simulations ends with  $n_S(T) = 1$  while the second half of simulations ends with  $n_S(T) = 0$ . Here  $n_S(T)$  denotes a final fraction of nodes in state  $S$ . The system prefers evolution toward  $n_S(T) = 1$  for points situated above this surface in  $(\mathcal{C}, p, n_S(0))$  space.

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The surface of the unstable fixed points in  $(\mathcal{C}, p, n_S(0))$  space.



## P33 – Threading dynamics of ring polymers in a gel

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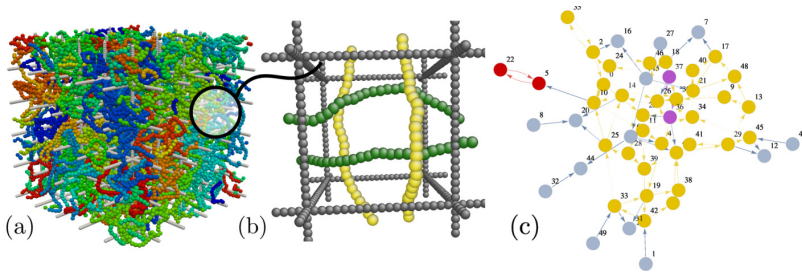
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Ring polymers continue to present a challenge to the theoretical community as the polymers lack of ends represents a severe topological constraint on their conformations, especially when diffusing through a gel. In particular, threadings between rings have always been conjectured to play an important role in solutions of closed chains, from the work of Klein [1] to more recent ones [2], but always proved very hard to detect and quantify. We performed large-scale Molecular Dynamics simulations of a concentrated solution of unknotted, unlinked rings in a background gel made up of a three dimensional cubic lattice of static polymer segments with lattice spacing equal to the chains Kuhn length (Fig. (a)), in order to detect inter-ring penetrations. We took advantage of the ordered architecture of our gel to unambiguously identify inter-ring threadings by measuring the linking of closed curves (Fig. (b)). We show that some of threadings have a life-time that is at least comparable to that of the longest relaxation time of the chains and argue that they may be much longer for longer chains than those we were able to simulate here. The achievement of an adequate description of inter-ring interactions could explain most of the confusion on the macroscopic properties of solutions of rings, where, on top of a fast diffusion, one can observe very long lived correlations. Finally, we compare our system to an evolving (directed) network of penetrating rings (Fig. (c)) and suggest that, in the limit of very long chains, a spanning connected component of threading rings may emerge, which would then exhibit very slow (glassy) dynamics at the scale of centre of mass motion for each chain, while retaining substantially unhindered motion at the level of individual chain segments. Having observed that the number of threadings per chain grows linearly with the length of the rings, we conjecture that such a topological glass is bound to emerge in the limit of very long rings.

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(a) Snapshot of our system. (b) Snapshot of the threading of two chains. (c) Snapshot of the directed network of inter-penetrating rings.

## P34 – Aging of downloads of scientific publications: a case study

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The history of web downloads of scientific publications in the journal “Europhysics Letters” (EPL) is analysed. Our initial motivation was to investigate whether there may be correlations between downloads and later citations, in order to check whether the former could play a predictive role for the later. But the analysis of aging of downloads is an interesting task in itself: while citations are usually considered as an indicator of academic impact, downloads reflect rather the level of attractiveness or popularity of a publication. This could be considered as a complementary measure to other scientometric measures, and for this reason we report on that here.

The statistics of downloads were analysed in two different ways (see [1]). While the so-called synchronous approach allows us to find patterns of downloads for different periods of a journal's life, the diachronous approach can be used to characterize the individual download histories of each paper. In particular, we found that, using the notions of half-life and of averaged cumulative numbers, it is possible to group EPL publications into several categories (e.g., see [2]). Similar to citations, downloads can accumulate in different ways: e.g., (i) in a typical manner, or (ii) slowly first, with with “bursts” later, or (iii) very actively at the beginning but

slowly later. The topic of current interest is to find the possible reasons for such different patterns of downloads which allows to classify scientific publications according to “popularity” or “exoticness” (“sleeping beauties” or “flash-in-the-pans”).

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## **P35 – Manipulating qubits by spin chain soliton excitations**

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Many proposals for quantum devices are based on qubits that are physically realized by the spin of quantum objects, such as atoms, molecules, quantum dots, and so on. The most adopted strategy for manipulating these qubits is that of applying suitable localized and time dependent magnetic fields. However, in solid-state based setups, selectively applying a field just to one qubit without disturbing the neighbouring ones is hardly attainable. In this work we propose to use magnetic solitons propagating along a spin chain to accomplish the above task. Indeed, if the chain is locally coupled with one qubit, as the soliton runs the qubit behaves, due to its interaction with the chain, as if it were subject to an effective magnetic field, well localized in space, whose time dependence is supplied by soliton's features. Moreover, the generation of solitons is proposed to be achieved by applying a proper magnetic field to one of the chain ends, which is considered far from the qubit we are interested in, when the whole system is initially aligned with a uniform magnetic field. We here present results for the time evolution of the qubit's density-matrix, whose dynamics is induced by the propagation along a classical Heisenberg chain of solitons of different shapes: this gives rise to different final

states proving the effectiveness of the above scheme in order to prepare and manipulate single qubits. In addition, we prove, by means of numerical simulations of the dynamics of spin variables of a classical discrete Heisenberg chain, the possibility of generating quite stable soliton-like excitations with the aforementioned method.

## P36 – Thermalization of low-dimensional quantum systems

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Statistical Mechanics was developed to explain the behavior of systems in the thermodynamic limit starting from a microscopic approach, i.e, its concepts are applied to systems with a large number of degrees of freedom. However, low-dimensional systems do not have such universally accepted concepts mainly because the Schrödinger's equation – responsible for the temporal evolution of quantum systems – is linear and the energy spectrum is discrete.

Classically, two systems are said to be in equilibrium when both of them have the same temperature. However, temperature is not well understood from the quantum mechanical point of view yet.

The *Eigenstate Thermalization Hypothesis* (ETH) [1] asserts that many-body quantum systems should thermalize regardless of its initial conditions before an observable (magnetization, occupation,...). Thus, the thermalization concept is associated with the temporal evolution of an observable.

As a suggestion, Gemmer and coauthors [2] proposed the spectral temperature

$$\frac{1}{k_B T} := - \left( 1 - \frac{W_0 + W_M}{2} \right)^{-1} \sum_{i=1}^M \left( \frac{W_i + W_{i-1}}{2} \right) \frac{\ln W_i - \ln W_{i-1} - \ln N_i + \ln N_{i-1}}{E_i - E_{i-1}} \quad (3)$$

where  $W_i$  is the probability of finding the quantum system in the energy level  $E_i$  and  $M$  is the number of levels.

This equation is derived from the maximization of Shannon's entropy

$$S = -k_B \sum_k W_k \ln W_k \quad (4)$$

once that classically the entropy is maximum when the system reaches equilibrium.

The objective of the present work is to present some results about thermalization and the spectral temperature of a finite quantum spin chain (Heisenberg XYZ) coupled with a gibbsian bath.

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## P37 – Contact processes with competitive dynamics in bipartite lattices: effects of distinct interactions

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The contact process (CP) with a competitive dynamics proposed by Martins *et al.* [Phys. Rev. E **84**, 011125 (2011)] leads to the appearance of an unusual active phase, in which the system sublattices are unequally populated. It differs from the usual CP only by the fact that particles also interact with their next-nearest neighbor sites via a distinct strength creation rate and for the inclusion of an inhibition effect, proportional to the local density. Aimed at investigating the robustness of such asymmetric phase, in this paper we study the influence of

distinct interactions. In the first model, the interaction between first neighbors requires a minimal neighborhood of adjacent particles for creating new offspring, whereas second neighbors interact as usual (e.g. at least one neighboring particle is required). The second model takes the opposite situation, in which the restrictive dynamics is in the interaction between next-nearest neighbors sites. Both models are investigated under mean field theory (MFT) and Monte Carlo simulations. In similarity with results by Martins *et al.*, the inclusion of distinct sublattice interactions maintains the occurrence of an asymmetric active phase and reentrant transition lines. In contrast, remarkable differences are presented, such as discontinuous phase transitions (even between the active phases), the appearance of tricritical points and the stabilization of active phases under larger values of control parameters. Finally, we have shown that the critical behaviors are not altered due to the change of interactions, in which the absorbing transitions belong to the directed percolation (DP) universality class, whereas second-order active phase transitions belong to the Ising universality class.

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## **P38 – Exact protein distributions for stochastic models of gene expression using partitioning of Poisson processes**

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Stochasticity in gene expression gives rise to fluctuations in protein levels across a population of genetically identical cells. Such fluctuations can lead to phenotypic variation in clonal populations, hence there is considerable interest in quantifying

noise in gene expression using stochastic models. However, obtaining exact analytical results for protein distributions has been an intractable task for all but the simplest models. Here, we invoke the partitioning property of Poisson processes to develop a mapping that significantly simplifies the analysis of stochastic models of gene expression. The mapping leads to exact protein distributions using results for mRNA distributions in models with promoter-based regulation. Using this approach, we derive exact analytical results for steady-state and time-dependent distributions for the basic 2-stage model of gene expression. Furthermore, we show how the mapping leads to exact protein distributions for extensions of the basic model that include the effects of post-transcriptional and post-translational regulation. The approach developed in this work is widely applicable and can contribute to a quantitative understanding of stochasticity in gene expression and its regulation.

## **P39 – Evolution of the magnetization after a local quench in the critical transverse-field Ising chain**

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We study the time evolution of the local magnetization in the critical Ising chain in a transverse field after a sudden change of the parameters at a defect. The relaxation of the defect magnetization is algebraic and the corresponding exponent, which is a continuous function of the defect parameters, is calculated exactly. In finite chains the relaxation is oscillating in time and its form is conjectured on the basis of precise numerical calculations.

## P40 – Controlled engineering of extended states in disordered systems

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We describe how to engineer wavefunction delocalization in disordered systems modelled by tightbinding Hamiltonians in  $d > 1$  dimensions. We show analytically that a simple product structure for the random onsite potential energies, together with suitably chosen hopping strengths, allows a resonant scattering process leading to ballistic transport along one direction, and a controlled coexistence of extended Bloch states and anisotropically localized states in the spectrum. We demonstrate that these features persist in the thermodynamic limit for a continuous range of the system parameters. Numerical results support these findings and highlight the robustness of the extended regime with respect to deviations from the exact resonance condition for finite systems. The localization and transport properties of the system can be engineered almost at will and independently in each direction. This study gives rise to the possibility of designing disordered potentials that work as switching devices and band-pass filters for quantum waves, such as matter waves in optical lattices.

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## P41 – Multifractal finite-size-scaling and universality at the Anderson transition

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We describe a new multifractal finite-size scaling (MFSS) procedure and its application to the Anderson localization-delocalization transition. MFSS permits the simultaneous estimation of the critical parameters and the multifractal exponents. Simulations of system sizes up to  $L^3 = 120^3$  and involving nearly  $10^6$  independent wave functions have yielded unprecedented precision for the critical disorder  $W_c = 16.530(16.524, 16.536)$  and the critical exponent  $\nu = 1.590(1.579, 1.602)$ . We find that the multifractal exponents  $\Delta_q$  exhibit a previously predicted symmetry relation and we confirm the nonparabolic nature of their spectrum. We explain in detail the MFSS procedure first introduced in our Letter [1] and, in addition, we show how to take account of correlations in the simulation data. The MFSS procedure is applicable to any continuous phase transition exhibiting multifractal fluctuations in the vicinity of the critical point.

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## P42 – Localisation and finite-size effects in graphene

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We show that electron states in disordered graphene, with an onsite potential that induces inter-valley scattering, are localised for all energies at disorder as small as 1/6 of the band width of clean graphene. We clarify that, in order for this Anderson-type localisation to be manifested, graphene flakes of size  $\approx 200 \times 200 \text{ nm}^2$  or larger are needed. For smaller samples, due to the surprisingly large extent of the electronic wave functions, a regime of apparently extended (or even critical) states is identified. Our results complement earlier studies of macroscopically large samples and can explain the divergence of results for finite-size graphene flakes.

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## P43 – Sampling low energy states of the Edwards-Anderson model

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The numerical search for ground states of the three-dimensional Edwards-Anderson spin glass with Gaussian bond distribution is very challenging and a variety of al-

gorithms have been introduced. So far, systems with sizes up to  $N \approx 12^3$  have been investigated by means of genetic methods. Here, we show how a competitive search algorithm can be designed when standard Monte Carlo techniques are combined with simple energy minimization procedures. In a second step we propose a modified Hamiltonian with an associated free energy landscape that contains the relevant minima, but can be sampled more efficiently.

## P44 – Jamming percolation in three dimensions

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Kinetically-constrained models have trivial interactions and relatively simple kinetic rules, which generate clusters of mutually-blocked particles, and thus lead to cooperative and slow relaxation; and ultimately to jamming when the typical size of these clusters exceeds the system size. The Kob-Andersen and Fredrickson-Andersen models, for which the kinetic constraint depends only on the number of neighboring occupied sites, have finite-sized blocked clusters at any particle density, and thus jam only in finite-sized systems. In jamming-percolation models, such as the spiral model, blocked particles form a system-spanning cluster at finite density, and thus exhibit an ergodic-nonergodic phase transition in the thermodynamic limit.

We generalized the spiral model to include density, temperature and nonequilibrium driving as separate control parameters, and disentangled the three different relaxation mechanisms responsible for unjamming when varying each of them [1]. Subsequently, we studied the effects of box size and shape on jamming in the Kob-Andersen and Fredrickson-Andersen models in arbitrary dimension [2, 3]. We showed how jamming can occur as the system's aspect ratio is changed, and find that the scaling laws for the critical density vs system size depend on the system's shape.

We will present our extension of jamming-percolation models to three dimensions [4]. We introduce a three-dimensional model, and prove that the fraction of frozen particles is discontinuous at the directed-percolation critical density. In agreement with the accepted scenario for jamming- and glass-transitions, this is a mixed-order transition; the discontinuity is accompanied by diverging length- and time-scales. Because one-dimensional directed-percolation paths comprise the backbone of frozen particles, the unfrozen rattlers may use the third dimension

to travel between their cages. Thus the dynamics are diffusive on long-times even above the critical density for jamming.

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## P45 – Superposition enhanced nested sampling

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Nested sampling is a Bayesian method for exploring arbitrary parameters spaces. In the context of statistical physics it can be used to directly and efficiently compute the density of states. As with other Monte Carlo based methods, nested sampling struggles when the energy landscape is very rugged, with large energy barriers separating thermodynamically important states. We report a new hybrid method for the exploration of systems exhibiting broken ergodicity on simulation time scales. Superposition enhanced nested sampling (SENS) combines the strengths of global optimisation algorithms with the unbiased/athermal sampling of nested sampling, greatly enhancing its efficiency with no additional parameters.

## P46 – Magnetization process of the spin-1/2 Ising-Heisenberg and Heisenberg tetrahedral chain: a comparison

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The frustrated spin-1/2 Ising-Heisenberg ladder with the Heisenberg intra-rung and Ising inter-rung interactions is exactly solved in a longitudinal magnetic field by taking advantage of the local conservation of the total spin on each rung and the transfer-matrix method. We have rigorously calculated the ground-state phase diagram, magnetization process, magnetocaloric effect and basic thermodynamic quantities for the model, which can be alternatively viewed as the Ising-Heisenberg tetrahedral chain. It is demonstrated that a stepwise magnetization curve with an intermediate plateau at a half of the saturation magnetization is also reflected in respective stepwise changes of the concurrence serving as a measure of bipartite entanglement. The ground-state phase diagram and zero-temperature magnetization curves of the Ising-Heisenberg tetrahedral chain are confronted with the analogous results of the purely quantum Heisenberg tetrahedral chain, which have been obtained through the extensive density-matrix renormalization group (DMRG) calculations. While both ground-state phase diagrams fully coincide in the regime of weak inter-rung interaction, the purely quantum Heisenberg tetrahedral chain develops Luttinger spin-liquid and Haldane phases for strongly coupled rungs, which are absent in the Ising-Heisenberg counterpart model.

## P47 – Multiferroicity in doped and undoped BTO-nanoparticles

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We investigate theoretically multiferroic material that possesses at least two coexisting ferroic orders in a single phase. Our analysis is based on the recent observation that typical ferroelectric materials such as BaTiO<sub>3</sub> (BTO) become multiferroic when it is prepared at the nanoscale. Nanoparticles (NP) composed of BTO offer at room-temperature magnetic hysteresis as well as temperature-dependent dielectric constant and a polarization. The magnetism in the nanoparticles (NP) has been suggested to be intrinsic and originates from cation or anion vacancies at the surfaces of the NP. Based on a microscopic Hamiltonian and a Green's function technique we demonstrate that the unexpected ferromagnetic properties of BTO-NP are due to oxygen vacancies at the surface of that material. Such vacancies lead to the appearance of Ti<sup>3+</sup> or Ti<sup>2+</sup> ions with nonzero net spin. The resulting different valence states composed of Ti-ions offer a nonzero magnetization which decreases with increasing particle size. The system shows a multiferroic behavior below a critical size of the nanoparticles and the related polarization tends to a saturation value when the particle size is enhanced. We have also analyzed the influence of magnetic fields and ion doping on the magnetic and electric properties in doped BTO.

## **P48 – Road traffic flow modeling and signal optimisation for fuel economy and emissions reduction in Coventry City based on experimental data**

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Nowadays, traffic congestion becomes a serious problem for many urban areas in the world. As the result of congestion, the efficiency of transportation infrastructure is generally reduced and a travel time is increased. Also, congestion creates the additional fuel consumption and generates air pollution.

The aim of projects carried out at Coventry University is to show how Intelligent Transport Systems (ITS) may be used in order to provide traffic improvement, air emissions reduction and fuel economy. The Ring Road and main roads in the Coventry City Centre have been created in a digital form for the computer simulation. Several tasks have been considered, i.e. modelling and simulation of an incident on the main road and the development of an alternative strategy to re-route the traffic; optimisation of existing traffic control plants in order to increase the traffic flow throughput and reduce pollutant emissions and fuel consumption; creating a flooding scenario in a Coventry Ring Road network in order to simulate the road traffic behavior at the time of flooding; and the addition of a traffic signal on a busy intersection, which allows one to reduce a stoppage time for vehicles and improve safety.

## **P49 – Entanglement via quantum repeated interactions**

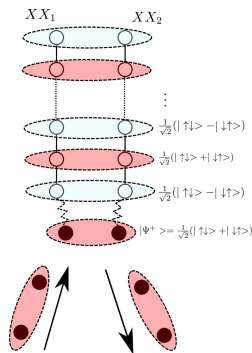
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We study the entanglement dynamics, via the concurrence, between spins belong-

ing to two different XX chains coupled on one edge to a quantum reservoir. This reservoir is modelled by an infinite set of Bell pairs, each constituent of the pairs interacting repeatedly with one chain only. The state of the whole system being Gaussian during the evolution, the system is characterized by means of two points fermionic correlations functions. We find that the steady state of the repeated interaction process leads to a steady state that is an alternation of maximally entangled states formed by pairs of spins belonging to the two chains.



## P50 – Specific interactions in a coarse-grained hard sphere model

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We use an off-lattice hard-sphere coarse grained model with a square well (sw) potential for studying structure formation of homopolymer chains [1]. Starting with tangent spheres, shortening of the bond length introduces stiffness. Due to this bond length reduction the spatial structure changed from crystalline to helical-like structures within the lower energy range of the density of states (DOS). We introduce a further interaction where predefined pairs interact via an additional sw potential. This allows the chain to reach lower energy states and leads to a stabilization of additional structures which will be shown in the analysis of thermodynamic functions. For an improved performance for estimating the DOS, the



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## **P51 – Gauge field for non-equilibrium processes and covariant version of Fisher information matrix**

**Takuya Yamano**

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The Fokker-Planck equation describes various non-equilibrium processes found in nature. It is recently pointed out that it can be expressed as a form of Fick's first law when we introduce a gauge field associated with the process, where the spatial gradient is replaced with the covariant derivative. The notion of Abelian gauge theory can be a useful approach for investigating the non-equilibrium Fokker-Planck equation, in which the associated curvature represents internal geometry.

In this presentation, by extending to a general nonlinear Fokker-Planck equation we show that the fluctuation of the gauge field in the process can be quantified with the Fisher information of the system. More specifically, we show that the fluctuation of the gauge field has three different origins. In the second part, we treat a Fisher information matrix by using a covariant derivative. The covariant version of the Fisher information matrix provides correlation between the flux component, however at the same time it raises a fundamental question as to whether or not the information should be gauge invariant [1, 2, 3].

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## P52 – Network analysis of medieval texts: Case study of the Battle of Clontarf (1014 AD)

**Joseph Yose, Ralph Kenna, Pádraig Mac Carron**

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*Cogad Gáedel re Gallaib* (the War of the Gaedhil with the Gaill) is a medieval text, the earliest version of which is dated to the 12th century. It tells of how an Irish army under the leadership of Brian Boru challenged Viking invaders who were in control of parts of the country. The narrative culminates with the Battle of Clontarf, which took place on Good Friday 23 April 1014, one millennium ago.

Until the 1970's many scholarly works about Vikings in Ireland accepted the accounts of *Cogad Gáedel re Gallaib* at face value. The events it describes entered the popular imagination as a straightforward tale of the Irish versus Vikings and the picture commonly portrayed is of Brian as of a great ruler who freed Ireland of Viking tyranny. Recent historical interpretations tell a more complex tale and the text is nowadays considered as quasi-history and propaganda to immortalise Brian Boru. The forces which opposed Brian included Leinster Irish and a rebellious Ulster regional king. Similarly, Brian's forces contained Viking contingents. The plethora of characters and social interactions makes the narrative an attractive one for the construction of a social network, especially in the light of the anniversary of events it purports to describe.

Here we perform an exploratory network analysis of the social relationships in the text, in the context of a broader sociophysics project applied to the humanities. We apply techniques from network theory to visualise the social network and investigate properties such as structural balance and community structure. We seek to address the question of how such a complex social landscape has persisted in the public imagination as a simple one of two homogeneous factions at war. Our poster is aimed at facilitating discussion around what questions can reasonably be asked and what, if anything, techniques from sociophysics can deliver.

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## P53 – Thermal properties of polymer knots.

Yani Zhao

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Polymer rings forming complex topological configurations are studied in connection with several applications ranging from biochemistry to mechanical engineering. The most difficult problem in dealing with the statistical mechanics of polymer knots is to distinguish their topological configurations. In this talk the results of polymer simulations of single polymer knots based on the Wang-Landau algorithm will be presented. To equilibrate the knots and for the Monte Carlo sampling, a set of pivot moves is used. To preserve the topology of the knots after each move, two recently developed techniques have been employed. One is the so-called PAEA method. It is able to detect the changes of topology exactly and is very fast. The other method is based on the Vassiliev knot invariant of degree 2 represented in the form of contour integrals. This invariant has the great advantage of allowing large pivot moves, which are able to accelerate the Monte Carlo sampling procedure. As an application of these methods, the calculation of the specific energy, the radius of gyration and the heat capacity of several types of knots will be presented. Some consequences on the thermodynamics of polymer knots will be drawn, like for example the existence of pseudo phase transitions from a collapsed state to an extended state. A comparison with the previously known result will be made.

- [1] Yani Zhao and Franco Ferrari, A numerical technique for studying topological effects on the thermal properties of knotted polymer rings, JSTAT (2012), P11022, arXiv 1209.1717.
- [2] Yani Zhao and Franco Ferrari, A numerical technique for preserving the topology of polymer knots: The case of short-range attractive interactions, Acta Physica Polonica B 44 (2013), 1193, arXiv:1212.6569.
- [3] Yani Zhao and Franco Ferrari, A study of polymer knots using a simple knot invariant consisting of multiple contour integrals, JSTAT (2013), P10010, arXiv:1306.5555.

## P54 – Path integral of twisted and bent DNA

Marco Zoli

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Complementary strands in DNA double helix show temporary fluctuational openings which are essential to biological functions such as transcription and replication of the genetic information. Such large amplitude fluctuations, known as the breathing of DNA, are generally localized and, microscopically, are due to the fact that the hydrogen bonds, linking the pair bases on the complementary strands, can break thus exposing the bases for chemical reaction. Theoretical approaches based on Hamiltonian methods are particularly advantageous in modeling the DNA dynamics as they can treat the system at the level of the base pairs incorporating nonlinear effects in heterogeneous sequences. I apply imaginary time path integral techniques to a mesoscopic Hamiltonian which accounts for the helicoidal geometry of short circular DNA molecules [1, 2]. The base pairs displacements with respect to the ground state are interpreted as time dependent paths. The portion of the paths configuration space contributing to the partition function is determined, at any temperature, by selecting the ensemble of path displacements whose amplitudes are consistent with the model potential for the hydrogen bonds. Helix unwinding and bubble formation patterns are computed in circular sequences with variable radius. Fluctuational openings appear along the helix to release the stress due to the bending of the molecule backbone [3]. The interplay between molecule size and appearance of helical disruptions is analyzed. The bubble probability profiles are compared to experimental data available for some minicircles.

- [1] M. Zoli, *J. Chem. Phys.* **135** (2011) 115101.
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- [3] M. Zoli, *J. Chem. Phys.* **138** (2013) 205103.

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## About Coventry

Coventry is a city in the county of west midlands in England and is well known for its rich history of industry. By the 14th century, Coventry was the fourth largest town in England with an estimated population of 8,000. It was an important centre of the cloth trade, and throughout the Middle Ages was one of the most important cities in England. In the 18th and 19th centuries, Coventry became one of the three main UK centres of watch and clock manufacture. In 1885 in Coventry, Rover produced the first bicycle to include modern features such as a chain-driven rear wheel with equal-sized wheels on the front and rear. By the 1890s the cycle trade was booming and Coventry had developed the largest bicycle industry in the world. To this day, the bicycle is called “Rover” in Poland and western Ukraine. The first British motor car was made in Coventry in 1897 by The Daimler Motor Company Limited. Coventry’s darkest hour came during World War II when it was singled out for heavy bombing raids. The symbol of the mythical phoenix, which the University has adopted is a reminder of the way in which the city of Coventry rebuilt itself after Second World War. Today the city is a centre of post-war reconciliation. Coventry is also known for the legendary 11th century Lady Godiva who, according to legend, rode through the city on horseback clothed only in her long hair, in protest of high taxes being levied on the cityfolk by her husband Leofric, Earl of Mercia.

## Pubs

Note that pubs and restaurants are two different species in England, although there are some hybrids. Traditionally, one goes to a pub to drink beer and relax with friends. Restaurants are for eating. Nowadays some pubs also serve food, typically nothing too fancy and not late in the evening. So, if you’re looking for decent nosh, skip to the restaurant section. Tipping is not expected in pubs (but it is in restaurants).

**Earl of Mercia:** *18 High street, CV1 5RE*

This pub caters for an older clientele. It has no piped music. It is cheap and cheerful and centrally located. They have a good selection of real ales and the quality is consistently very high. They serve cheap food which is also quite reasonable.

**Phoenix:** *122 Gosford Street, CV1 5DL*

This is a lively student venue nestled in Coventry University campus.

**Browns:** *Earl Street, CV1 5RU*

Browns is situated directly opposite the School of Art and Design. It has a wide, international selection of lagers and it is popular amongst the arty set. They also serve food.

**Whitefriars Olde ale House:** *114-115 Gosford Street, CV15DL*

Whitefriars is real ale pub in the centre of Coventry. They have a reasonable selection of ales, bitters and lagers, Pub food is available at lunchtimes throughout the week. Used to be a favourite amongst Coventry University staff but has declined a bit recently.

**Golden Cross:** *8 Hay Lane, CV1 5RF*

This is one of the oldest pubs in Coventry dating from 1583. It is reputed to be the most heavily haunted in the city. The structure of the building is typical of the Tudor-style with three vaulted or 'jettied' upper floors. Handy location in the city centre.

**The Establishment Bar & Grill:** *Bayley Lane, CV1 5RN*

Situated in the cobbled streets of the Cathedral Quarter, it is set in the old County Hall, which dates back to 1783. It was the main courthouse in Coventry up to the 1980's. The building is infamous as the place where the last hanging in Coventry took place. Features from the old courtroom have been beautifully restored, including the judge's seat, dock and viewing gallery.

**The Squirrel:** *Corner of Greyfriars Lane, CV1 2GY*

A clean, relaxing and comfortable place to unwind after a busy day. Tend to close early (about 9pm) during weekdays, however.

**Inspire Cafe Bar:** *New Union Street Coventry CV1 2PS*

A cafe bar located in one of Coventry's famous three spires. Quite small inside – but they have plenty of outside seating if the weather is OK. They also have a range of snacks which are reasonably priced. The beer is a bit on the expensive side, however and it only comes in bottles – no draught. The atmosphere is arty and bohemian.

## Restaurants

Coventry is a very multicultural city. If you are not from these parts, we recommend you try some of Coventry's excellent Indian and Chinese restaurants. It is reported that Britain's most popular dishes are the chicken tikka masala (Indian) and stir fry (Chinese). However, we also have excellent Arabic restaurants. Tipping is usual in restaurants (about 15%).

**Oriental Palace:** *27 London Road, CV1 2JP*

Tel: 024 76551533  
Cuisine: Chinese  
Our verdict: Excellent Chinese food at reasonable prices if you can ignore the outdated decor and style.

**Turmeric Gold:** *166 Medieval Spon Street, CV1 3BB*

Tel: 02476 226603  
Cuisine: Indian  
Our Opinion: Ranked number 5 in Coventry according to Tripadvisor. Highly recommended if you like spicy food.

**Pizza Express:** *10 Hay Lane*

Tel: +44 (0)24 7663 3156  
Cuisine: Italian  
Our Opinion: This is a chain. Drinks are very expensive but atmosphere is good and the pizzas are consistently good (for the UK – not by German or Italian standards).

**COSMO:** *36-42 Corporation Street, CV1 1GF*

Tel: 02476 553 366  
Cuisine: Pan-Asian  
Our Opinion: Buffet style – all you can eat. Reasonably priced, friendly efficient staff. Very good for large groups.

**Aqua Food and Mood Restaurant:** *14 The Butts, CV1 3GR*

Tel: 024 7622 9551  
Cuisine: Lebanese. Halal.  
Our Opinion: Excellent.

**Bella Italia Restaurant:** *4 Belgrade Plaza, Upper Well Street, CV1 4BF*

Tel: 024 7622 6811  
Cuisine: Italian.  
Our Opinion: Reasonably prices, comfortable. Nice atmosphere.

**Browns Cafe:** *Earl Street, CV1 5RU*

Tel: 024 7622 1100  
Cuisine: Coffee & Various.  
Our Opinion: This is a hybrid – part pub, part restaurant.

**China Red Restaurant:** *58 Hertford Street, CV1 1LB*

Tel: 024 7622 9333  
 Cuisine: Chinese  
 Our Opinion: Authentic Chinese.

**Habibi's Restaurant:** *142 Far Gosford Street, CV1 5DY*

Tel: 024 7622 0669  
 Cuisine: Arabic.  
 Our Opinion: Halal restaurant – very high quality food and well worth a visit. They don't serve alcohol but you can buy beer or wine at one of the shops nearby (which are open late) and bring with you to the restaurant.

**Thai Dusit Restaurant:** *39 London Road, CV1 2JR*

Tel: 024 7622 7788  
 Cuisine: Thai  
 Our Opinion: Good quality Thai restaurant. Slightly more expensive than average for Coventry.

## Safety and emergency numbers

999	in emergencies to contact the Police, Fire or Ambulance
112	emergency services anywhere in the EU
0345 113 5000	Coventry Police (for non-emergencies)

## Hospitals

University Hospital (Coventry)  
 Clifford Bridge Road, Coventry,  
 West Midlands, CV2 2DX

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[www.uhcv.nhs.uk](http://www.uhcv.nhs.uk)

Opening Times: Every day – 24 hours



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Locations

Please consult the map overleaf for the most important MECO39 locations:

- A Applied Mathematics Research Centre at the Design Hub**
- B Engineering and Computing Building: main conference site**
- C Ibis Hotel Coventry Centre**
- D Ramada Hotel & Suites**
- E Coventry main station**
- F The Establishment Bar & Grill: welcome drinks on Monday April 7th**

