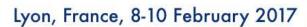


MECO 42

42nd Conference of the Middle-European Cooperation in Statistical Physics





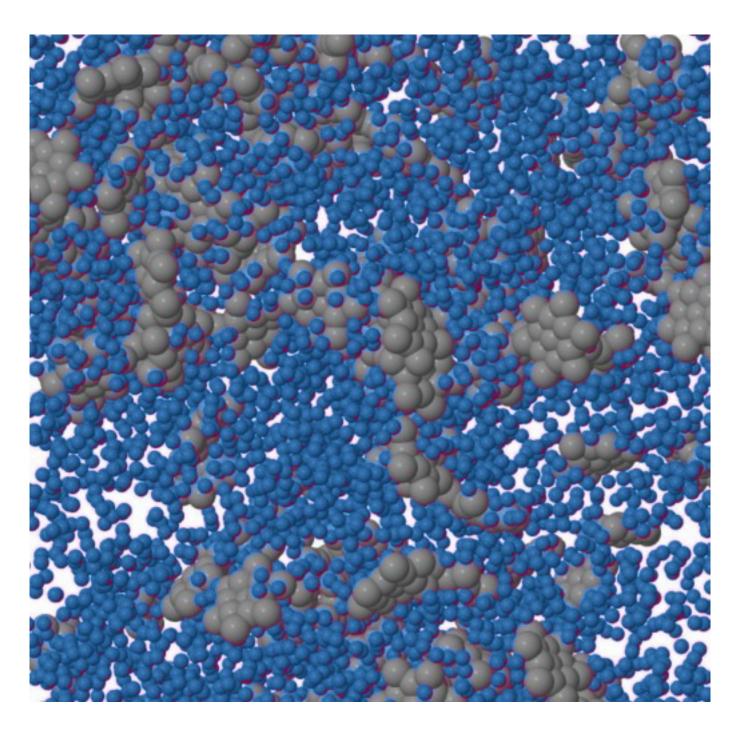


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Programme

8:00 -	Registration - Welcome of the participants
9.00	Registration - welcome of the participants

Session I: Soft matter and biophysics

9:00 – 9:50	Annette Zippelius	Dense Granular Flow
9:50 - 10:10	Wolfhard Janke	Free-Energy Barriers: From Particle Condensation to Polymer Aggregation
10:10 - 10:30	Kirill Polovnikov	Two-point correlations in chromosome loci dynamics: chain packing effects vs. viscoelastic surrounding media
10:30 - 11:00		Coffee break

Session II: Soft matter and biophysics

11:00 - 11:40	Emanuela Zaccarelli	Anomalous slow dynamics in soft matter
11:40 - 12:00	Fred Hucht	The square lattice Ising model on the rectangle
12:00 - 12:40	Sergio Ciliberto	A protocol for reaching equilibrium arbitrary fast
13:00 - 14:30		Lunch

Session III: Quantum many-body systems

14:30 - 15:20	Zoran Hadzibabic	Quantum gas in a box
15:20 - 15:40	Giuseppe Carleo	Solving the Quantum Many-Body Problem with Artificial Neural Networks
15:40 - 16:00	Ferenc Igloi	Critical quench dynamics of random quantum spin chains
16:00 - 16:30		Coffee break

Session III: Machine learning & Neural networks

16:30 - 17:10	Lenka Zdeborova	Spectral analysis of sparse data: Translating physics into algorithms
17:10 - 17:30	Mariana Krasnytska	Critical behavior on complex networks: inhomogeneous mean-field vs Lee-Yang-Fisher formalism
17:30 – 17:50	Carlo Lucibello	Probing the energy landscape of neural networks
17:50 – 18:10	Eytan Katzav	Analytical results for the distribution of shortest path lengths in random networks
18:10 - 19:00		Cocktail

Session IV: Quantum out-of-equilibrium systems

9:00 - 9:50	Jean-Sébastien Caux	Dynamics and relaxation in integrable quantum systems
9:50 - 10:10	Laura Foini	Measuring effective temperatures in a generalized Gibbs ensemble
10:10 - 10:30	Viktor Eisler	Universal front propagation in the quantum Ising chain
10:30 - 11:00		Coffee break

Session V: Disordered quantum systems

11:00 - 11:40	Peter Prelovsek	Many-body localization in disordered spin and Hubbard chains
11:40 – 12:00	Piotr Sierant	Many-body localization due to random interactions
12:00 - 12:20	Alessandro Cuccoli	Dynamics of hybrid quantum systems
12:20 - 12:40	Robert Whitney	Non-Markovian quantum thermodynamics: second law and fluctuation theorems
13:00 - 14:30		Lunch

Session VI: Active matter

14:30 - 15:20	Irene Giardina	Information propagation and collective swings in biological groups
15:20 – 15:40	Guillaume Briand	Crystallization of self-propelled hard-discs : a new scenario
15:40 – 16:10		Coffee break

Session VII: Interdisciplinary topics

16:10 - 16:30	Debarghya Banerjee	Odd viscosity in chiral active liquids
16:30 – 16:50	Kenneth Golden	Statistical physics and melting Arctic sea ice
16:50 - 17:10	Freddy Bouchet	Large deviation theory applied to climate physics, a new frontier of statistical physics
17:10 – 17:15	Zdzislaw Burda	Presentation of the MECO43
17:15 – 18:30		Poster session
18:30 - 21:00		Conference dinner

Programme Friday 10.02.17

Session VIII: Classical out-of-equilibrium systems

9:00 - 9:50	Peter Sollich	Non-affine fluctuations and pleating transitions in crystalline solids
9:50 - 10:10	Jacopo De Nardis	Memory and universality in interface growth
10:10 - 10:30	Alessio Chiocchetta	Dynamical crossovers in prethermal critical states
10:30 - 11:00		Coffee break

Session IX: Disordered classical systems

11:00 - 11:40	Kay J. Wiese	The Field theory of avalanches
11:40 - 12:00	Kirsten Martens	A statistical physics approach for the flow transition of yield stress fluids
12:00 - 12:20	Ivan Balog	Hysteresis in the random-field Ising model
12:20 - 12:40	Tadeusz Kopeć	Sherrigton-Kirkpatrick glassy-phase of random Josephson coupled Bose-Einstein condensates in wood-pile geometry
13:00 – 14:30		Lunch

Session X: Frustrated systems & Topological phases

14:30 - 15:10	Virginie Simonet	Magnetic charge injection in spin ice
15:10 – 15:30	Stephen Powell	Quantum Kasteleyn transition
15:30 - 15:50	Michele Modugno	Simulating condensed matter with ultracold atoms: the Haldane model and the Peierls substitution
15:50 - 16:40	John Chalker	Classical loop models and quantum magnets
16:40 – 17:30		Farewell Coffee







ED 52 - PHAST Physique & Astrophysique de Lyon











History of the MECO conferences

The Conferences of the Middle European Cooperation in Statistical Physics (MECO) were initiated in 1974 with the aim of bridging the gap between the communities of scientists from the Eastern and Western blocks of Europe, separated by the iron curtain. Since then, MECO conferences have become the yearly itinerant reference meetings for the community of scientists who are active in the field of Statistical Physics in the broader sense, including modern interdisciplinary applications to biology, finance, information theory, and quantum computation. The conference organized in Lyon in 2017 is the 42nd in the series of MECO meetings.

The previous MECO conferences were held in

1974	Wien (A)	1975	Regensburg (FRG)
1976	Bled (Y)	1977	Unterageri (CH)
1978	Boszkowo (PL)	1979	Trieste (I)
1980	Budapest (H)	1981	Saarbrucken (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	Balatonfured (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-à-Mousson (F)	2001	Prague (CZ)
2002	Sopron (H)	2003	Saarbrucken (D)
2004	Bratislava (SK)	2005	Cortona (I)
2006	Primosten (CR)	2007	Ladek Zdroj (PL)
2008	Puchberg/Wels (A)	2009	Leipzig (D)
2010	Pont-à-Mousson (F)	2011	Lviv (UA)
2012	Tatrianske Matliare (SK)	2013	Trieste (I)
2014	Coventry (UK)	2015	Esztergom (HU)
2016	Wien (A)	2017	Lyon (F)

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Scope of the 42nd edition

The 42nd meeting is addressed to both theoreticians and experimentalists working in the broad domains of Statistical Mechanics and Condensed Matter Physics. It is focused mainly but not exclusively on:

- Disordered systems
- Quantum many body systems
- Frustrated systems
- Topological phases of matter
- Non-equilibrium phenomena
- Active matter
- Soft matter and biophysics

Local Organizing Committee

Thierry Biben (Université Claude Bernard Lyon 1)
Andrei Fedorenko (ENS de Lyon)
Peter Holdsworth (ENS de Lyon)
Edmond Orignac (ENS de Lyon)
Tommaso Roscilde (ENS de Lyon)

Venue

The conference will take place at the Jacques Monod site of the Ecole Normale Supérieure de Lyon. It is situated in the Gerland area of the 7th district of Lyon (ENS de Lyon 46, allee d'Italie F69007 LYON). All invited and contributed talks will take place in the "Amphithéâtre Charles Mérieux", which has a capacity for an audience of 511 people. Posters will be displayed in the Atrium of the amphitheater.

Registration

Registration of the participants will start in the Atrium on Wednesday, 8th of February, at 8:00. The opening of the conference is scheduled at 9:00.

Coffee breaks, lunches, welcome cocktail and conference dinner

All coffee breaks during the conference will be delivered on site. Lunches on Wednesday and Thursday will take place at the Resto'U ENS Monod situated next to the amphitheater. Lunch boxes will be delivered on site on Friday, 10th of February. A welcome cocktail will be served in the Atrium on Wednesday, 8th of February, at 18:10. The conference dinner will take place in the Atrium on Thursday, 9th of the February at 18:30. Lunches, coffee breaks, welcome cocktail and the conference dinner are free of charges for all registered participants.

Further Information

The official site: https://meco42.sciencesconf.org

Emails: meco42@sciencesconf.org and meco42@ens-lyon.fr

MECO42

Invited Oral Presentation

Dense Granular Flow

Annette Zippelius

Institut fur Theoretische Physik - Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

A jamming scenario of frictional particles is discussed and interpreted in terms of a nonequilibrium first order phase transition [1]. Results of numerical simulations will be presented and analyzed in the framework of a simple model which can account for both, the continuous frictionless case and the discontinuous frictional case. The most important features of the frictional phase diagram are reentrant behavior and a critical jamming point at finite stress. In the simulations, we observe that small systems settle into a stationary state, whereas large systems do not relax to a stationary state on the timescale of observation, but rather display chaotic time dependence [2]. We propose a hydrodynamic model which couples stress relaxation to a scalar variable accounting for the microstructure of the packing. Linear stability analysis reveals an extended phase diagram which in addition to regions of stationary flow and jammed states displays chaos. We also develop a microscopic picture of reentrant flow and shear thickening, which emphasizes the role of friction.

[1] M. Grob, C. Heussinger, and A. Zippelius, Phys. Rev. E89, 050201 (R) (2014).

[2] M. Grob, A. Zippelius and C. Heussinger, Phys. Rev. E93, 030901 (R) (2015).

Anomalous slow dynamics in soft matter

Emanuela Zaccarelli

CNR-ISC: Institute of Complex Systems and Dipartimento di Fisica Universita' "La Sapienza" Rome, Italy

Dynamic arrest in soft matter systems manifests in a variety of arrested states, including gels, attractive and repulsive glasses. Usually, the approach to an arrested state happens through a two-step relaxation of the dynamic auto-correlation functions, where the microscopic, fast relaxation is separated from the structural, slow relaxation by an intermediate plateau often interpreted in terms of the so-called cage effect. However, anomalous dynamics where this picture in not valid is observed in many situations for soft matter systems. In this case, the two-step behavior is replaced by a logarithmic relaxation of the density auto-correlation functions, which is accompanied by a sub-diffusive behavior of the mean-squared displacement. In this talk I will present some examples of anomalous slow dynamics in simulations and experiments, and I will discuss the current theoretical understanding of this behavior.

MECO42

A protocol for reaching equilibrium arbitrary fast

Sergio Ciliberto

Laboratoire de Physique, UMR5672, École Normale Supérieure (ENS) - Lyon – 46 allée d'Italie 69007 Lyon, France

When a control parameter of a system is suddenly changed, the accessible phase space changes too and the system needs its characteristic relaxation time to reach the final equilibrium distribution. An important and relevant question is whether it is possible to travel from an equilibrium state to another in an arbitrary time, much shorter than the natural relaxation time. Such strategies are reminiscent of those worked out in the recent field of Shortcut to Adiabaticity, that aim at developing protocols, both in quantum and in classical regimes, allowing the system to move as fast as possible from one equilibrium position to a new one, provided that there exist an adiabatic transformation relating the two. Proof of principle experiments have been carried out for isolated systems. Instead in open system the reduction of the relaxation time, which is frequently desired and necessary, is often obtained by complex feedback processes.

In this talk, we present a protocol,named Engineered Swift Equilibration (ESE), that shortcuts time-consuming relaxations. We tested experimentally this protocol on a Brownian particle trapped in an optical potential first and then on an AFM cantilever. We show that applying a specific driving, one can reach equilibrium in an arbitrary short time. We also estimate the energetic cost to get such a time reduction. Beyond its fundamental interest, the ESE method paves the way for applications in micro and nano devices, in high speed AFM, or in monitoring mesoscopic chemical or biological process.

- [1] Ignacio A Martinez, Artyom Petrosyan, David Guéry-Odelin, Emmanuel Trizac, Sergio Ciliberto, "Engineered Swift Equilibration", Nature Physics, 12, 843 (2016).
- [2] Anne Le Cunuder, Ignacio A Martinez, Artyom Petrosyan, David Guéry-Odelin, Emmanuel Trizac, Sergio Ciliberto, "Arbitrary fast modulation of an atomic force microscope", Applied Physics Letters, 109, 113502 (2016).

Quantum gas in a box

Zoran Hadzibabic

Cavendish Laboratory - University of Cambridge - Astrophysics Group Department of Physics Cavendish Laboratory University of Cambridge The Old Schools Trinity Lane Cambridge CB2 1TN, United Kingdom

For the past two decades harmonically trapped ultracold atomic gases have been used with great success to study fundamental many-body physics in a flexible experimental setting. In 2013 we created the first atomic Bose-Einstein condensate (BEC) in an essentially uniform potential of an optical box trap [1]. Compared to the traditional setting of a harmonic trap, this has opened new possibilities for closer connections with other many-body systems and the theories that rely on the translational symmetry of the system. I will give an overview of our recent experiments on this system, including studies of the (Kibble-Zurek) dynamics of spontaneous symmetry breaking [2] and the emergence of turbulence in a periodically driven gas [3].

- [1] A. L. Gaunt et al., PRL 110, 200406 (2013).
- [2] N. Navon et al., Science 347, 167 (2015).
- [3] N. Navon et al., Nature 539, 72 (2016).

Spectral analysis of sparse data: Translating physics into algorithms

Lenka Zdeborova

Institut de Physique Théorique (ex SPhT) (IPHT) – CEA, CNRS : URA2306 – Institut de Physique Théorique Orme des Merisiers batiment 774 Point courrier 136 CEA/DSM/IPhT, CEA/Saclay F-91191 Gif-sur-Yvette Cedex, France

A number of problems in data science can be solved using algorithms based on the spectrum of a matrix associated with the data. Principal component analysis is a well-known example of such a spectral method. There are many examples of applications that require the matrix associated with the data to be sparse. However, the traditionally considered sparse matrices associated to the data develop spurious large eigenvalues associated with localised eigenvectors that harm the algorithmic performance. These so-called Lifshitz tails are analogous to impurity states in disordered systems. Inspired by the theory of spin glasses, we introduce the non-backtracking operator that is able to mitigate this problem and has no spurious eigenvalues. We discuss properties of this operator, as well as its applications to several algorithmic problems such as clustering of networks, percolation, matrix completion or inference from pairwise comparisons.

Dynamics and relaxation in integrable quantum systems

Jean-Sébastien Caux

Institute for Theoretical Physics, University of Amsterdam, Science Park 904, 1098 XH, Amsterdam – Netherlands

Recent years have witnessed rapid progress in the use of integrability in characterizing the out-of-equilibrium dynamics of low-dimensional systems such as interacting atomic gases and quantum spin chains. This talk will provide an introduction to these developments, with a particular focus on the Quench Action method. Exact solutions to the interaction turn-on quench in the Lieb-Liniger model and to the Néel-to-XXZ quench in spin chains will be presented. Particular emphasis will be given to interesting open issues and challenges, including the failure of the (local) Generalized Gibbs Ensemble to properly describe post-quench steady-state properties and the necessity to include quasilocal conserved charges to obtain correct answers.

Many-body localization in disordered spin and Hubbard chains

Peter Prelovsek

Jozef Stefan Institute and Faculty of Mathematics and Physics, University of Ljubljana – Slovenia

The many-body localization (MBL) is the quantum phenomenon involving the interplay of disorder and particle interaction, characterized mainly by the non-ergodic behavior. Recently it is intensively investigated theoretically within one-dimensional many-body models, and experimentally in optical lattices of cold atoms, but might be relevant also for materials with spin chains. In the talk the evidence for the transition to the MBL will be presented as it emerges from numerical investigations on the one-dimensional disordered spin and Hubbard models. It will be shown that within a random-eld spin chain dynamical staggered correlations, which are frequently used as the order parameter for the MBL phase, are closely related to the uniform dynamical spin conductivity and d.c. transport, whereby the transition is best characterized by the universal critical dynamics. On the other hand, an analogous numerical investigation of the disordered Hubbard chain indicates that disordered potential does not induce full MBL, but only charge localization while spin correlations vanish for large times.

Information propagation and collective swings in biological groups

Irene Giardina

Dipartimento di Fisica, Universita' di Roma La Sapienza, P. A. Moro 2, 00185 Rome, Italy

Collective changes in biological groups require all individuals in the group to go through a behavioral change of state. Sometimes these changes are triggered by external perturbations, as in evasive maneuvers of animal groups under predatory attacks. Often, however, they occur spontaneously and are only due to internal behavioral fluctuations. In all cases, the efficiency of information transport is a key factor to prevent cohesion loss and preserve collective robustness. In this talk, I will present an experimental and theoretical study of collective movements in animal groups. Starting from experimental data on collective turns in starling flocks, I will discuss what is the mechanism that triggers a collective change (a turn) and grants efficient and fast information propagation through the system. Finally, I will discuss the role of heterogeneities, network unbalance, and boundary effects in initiating a collective change of state.

Non-affine fluctuations and pleating transitions in crystalline solids

Peter Sollich

King's College London - WC2R 2LS London, United Kingdom

I will review our recent attempts to understand the equilibrium and non - equilibrium behaviour of non-affine fluctuations in solids. We measure local non-affinity χ by a systematic coarse graining of microscopic atomic displacements. This generates a local elastic deformation tensor D and the non-affinity as the extent to which the displacements are not representable as affine deformations of a reference crystal. We calculate the statistics of χ and D and their spatio-temporal correlations for solids at low temperatures, within a harmonic approximation. The calculation allows us to identify the dominant non-affine fluctuation modes, which have an interpretation as precursors for the nucleation of lattice defects.

In a second part I describe a phase transition that results when total non-affinity is biased by an appropriate conjugate field, in a two-dimensional network solid. Monte Carlo simulations reveal that the network supports, apart from the homogeneous phase, a "pleated" phase that has stress localised in rows of pleats and eliminated from the rest of the lattice. The kinetics of the phase transition is extremely slow in molecular dynamics simulation near coexistence, due to very large free energy barriers. When the external field is increased beyond coexistence to lower these barriers, the network exhibits rich dynamic behaviour: it transforms into a metastable phase with the stress now localised in a disordered arrangement of pleats. The pattern of pleats shows ageing dynamics and slow relaxation to equilibrium. Our predictions should be amenable to experimental testing using tethered colloidal solids in dynamic laser traps.

- [1] S. Ganguly, S. Sengupta, P. Sollich, and M. Rao, Phys. Rev. E 87, 042801 (2013).
- [2] S. Ganguly, S. Senguptab and P. Sollich Soft Matter 11, 4517 (2015).
- [3] A. Mitra, S. Ganguly, S. Sengupta, and P. Sollich, JSTAT P06025 (2015).
- [4] S. Ganguly, J. Horbach, P. Sollich, P. Nath, S. Karmakar, and S. Sengupta arXiv:1612.00574 (2016).

The Field theory of avalanches

Kay Wiese

Laboratoire de Physique Théorique de l'ENS (LPTENS) – CNRS : UMR8549, Université Pierre et Marie Curie (UPMC) - Paris VI, École normale supérieure [ENS] - Paris – 24 rue Lhomond, 75231 Paris CEDEX 05, France

When elastic systems like contact lines on a rough substrate, domain walls in disordered magnets, or tectonic plates are driven slowly, they remain immobile most of the time, before responding with strong intermittent motion, termed avalanche. I will describe the field theory behind these phenomena, explain why its effective action has a cusp, and how such intricate objects as the temporal shape of an avalanche can be obtained. Finally, an exact mapping to the Manna sandpile model is discussed.

Magnetic charge injection in spin ice

Virginie Simonet ¹, Emilie Lefrançois ², Vadim Cathelin ¹, Julien Robert ¹, Elsa Lhotel ¹, Rafik Ballou ¹, Laurent Chapon ³, Pascal Lejay ¹, Françoise Damay ⁴, Claire Colin ¹, Jacques Ollivier ², Bjorn Fak ²

¹ Institut Néel (NEEL) – CNRS : UPR2940 – 25 rue des Martyrs - BP 166 38042 GRENOBLE CEDEX 9, France

The spin ice state emerges in pyrochlore lattices of vertex sharing tetrahedra when the magnetic moments are subjected to an effective ferromagnetic interaction and are constrained along the local directions joining the corners to the center of each tetrahedron. It is a macroscopically degenerate ground state called a Coulomb phase, in which the spins obey locally the ice-rule, which means that two spins point in and two spins point out of each tetrahedron. The spin ice elementary excitations, the magnetic monopoles, are obtained by reversing one spin at the center of a pair of tetrahedra.

We propose a new mechanism to inject monopoles in a spin ice through a staggered magnetic field. We show experimentally that this is realized in a rare-earth pyrochlore iridate where the iridium sublattice produces, at the rare-earth site, a staggered magnetic field, pointing inwards/outwards adjacent tetrahedra. A new peculiar ground state is stabilized originating from the competition between the antiferromagnetic-like molecular field and the ferromagnetic spin-ice correlation. Compared to conventional spin ices, the different nature of the excitations in this new state opens the way to novel field-induced and dynamical behaviors.

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 ³ Diamond – Didcot, Oxfordshire, United Kingdom, United Kingdom
 ⁴ Laboratoire Léon Brillouin (LLB - UMR 12) – CEA, CNRS : UMR12 – LLB - UMR 12, CEA
 Saclay 91191 GIF SUR YVETTE CEDEX, France

Classical loop models and quantum magnets

John Chalker

Theoretical Physics, University of Oxford – 1 Keble Road, Oxford OX1 3NP, United Kingdom

I will give an overview of recent work on the statistical physics of lattice models of close-packed loops and their relation to quantum magnets. These models describe a number of problems in classical statistical physics – where, for example, the loops may be vortex lines in a three-dimensional random field – and also in antiferromagnets – where the loops are world-lines of quantum particles. The loop models have two phases – one in which all loops are finite, and another in which some loops are extended – corresponding ground states of an antiferromagnet with respectively valence bond and Néel order. I will discuss the continuum description of these systems and present results from Monte Carlo simulations. In particular, these loop models are a convenient way to access the transition from the valence bond solid to a Néel states, which is a candidate deconfined critical point.

Contributed Oral Presentations

Free-Energy Barriers: From Particle Condensation to Polymer Aggregation

Wolfhard Janke, Johannes Zierenberg, Philipp Schierz

Universität Leipzig, Institut für Theoretische Physik (ITP) – Postfach 100920, 04009 Leipzig, Germany

We present a new methodology to study temperature-driven droplet formation for both particle and polymer systems [1]. In particular, this allows a shape-free determination of the free-energy barrier. Combined with rigorous results on equilibrium droplet formation of particles, this enables a well-defined finite-size scaling analysis of the free-energy barrier at fixed density. We verify our theoretical predictions using parallel multicanonical Monte Carlo simulations [2] of a Lennard-Jones particle gas and generalize this approach to aggregation in a dilute bead-spring polymer solution. Our results suggest an analogy between polymer aggregation and particle condensation, when the macromolecules are interpreted as extended particles. We will briefly comment on the role of kinetic energy on the free-energy barrier, which is commonly neglected in Monte Carlo simulation studies [3].

- [1] J. Zierenberg, P. Schierz, and W. Janke, Canonical Free-Energy Barrier of Particle and Polymer Cluster Formation, Leipzig preprint (March 2016), arXiv:1607.08355 [cond-mat.stat-mech].
- [2] J. Zierenberg, M. Marenz, and W. Janke, Scaling Properties of a Parallel Implementation of the Multicanonical Algorithm, Comput. Phys. Commun. 184 (2013) 1155.
- [3] P. Schierz, J. Zierenberg, and W. Janke, First-Order Phase Transitions in the Real Microcanonical Ensemble (Editors' Suggestion), Phys. Rev. E 94 (2016) 021301(R).

Two-point correlations in chromosome loci dynamics: chain packing effects vs. viscoelastic surrounding media

Kirill Polovnikov ^{1,2}, Mike Tamm ^{3,1}

¹ Physics Department, Moscow State University – Russia

In recent years there have seen plethora of new theoretical and experimental studies of chromosome structure and dynamics, both in eukaryotic and prokaryotic cells. Combination of theoretical considerations (e.g., necessity that chromosome parts disentangle easily during the transcription) and experimental observations (presence of distinct chromosome territories, locus-locus contact maps obtained by the Hi-C method) make us believe that at least in many cases spatial organization of chromosome is self-similar on different lengthscales, and resembles the so-called fractal globule. Study of the chromosome matter dynamics provides important information about DNA organization, and is crucial in order to understand the functioning of the cell machinery. Contemporary single-particle tracking techniques have allowed to study the statistics of loci displacements in both eukaryotic and prokaryotic cells, in both cases the statistics of these displacement seems to be well described by fractal Brownian motion with Hurst exponent close to 0.2, which is significantly different from the exponent 0.25 predicted by the classical Rouse model of polymer dynamics. In literature, there exist at least two competing explanations for this slower-than-Rouse subdiffusion: either it is caused by the viscoelastic properties of the surrounding intra-cellular medium [1], or by the non-Gaussian packing of the chromosome into a fractal globule [2]. Here we present a theoretical framework which allows us to unify these two possible explanations and calculate the locus-locus correlation functions for a polymer chain (chromosome) packed in a fractal state with arbitrary fractal dimension and surrounded by viscoelastic medium whose dynamics is described by the generalized Langevin equation. Our results are a direct generalization of those obtained in [3] for a Gaussian chain in viscoelastic media, and we use the beta-model suggested in [4] to model polymer conformations with arbitrary fractal dimensions. We show that the presence of viscoelastic media does not change the fractal dimension of the equilibrium polymer conformation, but simply slows down the relaxation in the system. The characteristic relaxation times of the chain are calculated and concrete forms of correlation decay functions obtained. As a result, we suggest a theoretical framework allowing to distinguish between the effects of topological interactions (fractal dimension) and influence of media viscoelasticity (memory), and provide a way to recover both fractal dimension of packing and the characteristics of the viscoelastic media from the results of experiments on one-point and two-point DNA locus tracking.

[1] S. C. Weber, J. A. Theriot, A. J. Spakowitz, Physical Review E, 82, 011913

² Skolkovo Institute of Science and Technology – Russia

³ Department of Applied Mathematics, National Research University Higher School of Economics – Russia

(2010).

- [2] M.V. Tamm, L.I. Nazarov, A.A. Gavrilov, A.V. Chertovich, Phys. Rev. Letters, 114, 178102 (2015).
- [3] T. J. Lampo, A. S. Kennard, A. J. Spakowitz, Biophysical Journal, 110, 338 (2016).
- [4] A. Amitai, D. Holcman, Physical Review E, 88, 052604 (2013).

The square lattice Ising model on the rectangle

Fred Hucht

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The partition function of the square lattice Ising model on the rectangle is calculated exactly for arbitrary system size $L \times M$ and temperature. We start with the dimer method of Kasteleyn, McCoy & Wu, construct a highly symmetric block transfer matrix and derive a factorization of the involved determinant, effectively decomposing the free energy of the system into two parts, where the subleading residual part contains the nontrivial finite-L contributions for fixed M. It is given by the determinant of a $M/2 \times M/2$ matrix and can be mapped onto an effective spin model with M Ising spins and long-range interactions. While the residual part becomes exponentially small for large L/M or off-critical temperatures, it leads to important finite-size effects such as the critical Casimir force near criticality.

In the finite-size scaling limit, the involved expressions simplify and lead to the scaling functions of the Casimir potential and of the Casimir force. At criticality, a prediction from conformal field theory is confirmed.

- [1] Alfred Hucht, "The square lattice Ising model on the rectangle I: Finite systems", J Phys A: Math. Theo., 2016, arXiv:1609.01963 (accepted).
- [2] Alfred Hucht, "The square lattice Ising model on the rectangle II: Finite-size scaling limit" (in preparation).

Solving the Quantum Many-Body Problem with Artificial Neural Networks

Giuseppe Carleo ¹, Matthias Troyer ^{1,2,3}

The challenge posed by the many-body problem in quantum physics stems from the difficulty of describing the non-trivial correlations encoded in the wave function. In principle, an exponential amount of information is needed to fully characterize a generic many-body quantum state. However, it is often the case that a wave function representing a physical many-body system can be characterized by an amount of information much smaller than the maximum capacity of the corresponding Hilbert space. This leads to the enourmous success of numerical methods either aiming at sampling (Quantum Monte Carlo) or compressing (Tensor Network methods) the many-body state. The existing methods however suffer from limitations (sign problem for Quantum Monte Carlo, and dimensionality for Tensor Networks) which strongly limit the physical systems we can explore. In our work we demonstrate that an alternative route is viable. We show that systematic machine learning of the wave function can reduce the exponenentialy complexity of the wave-function to a tractable computational form, for some notable cases of physical interest. We introduce a variational representation of quantum states based on artificial neural networks with variable number of hidden neurons. A reinforcement-learning scheme is then demonstrated, capable of either finding the ground-state or describing the unitary time evolution of complex interacting quantum systems. We show that this approach achieves very high accuracy in the description of equilibrium and dynamical properties of prototypical interacting spins models in both one and two dimensions, thus offering a new powerful tool to solve the quantum many-body problem.

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Critical quench dynamics of random quantum spin chains

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By means of free fermionic techniques combined with multiple precision arithmetic we study the time evolution of the average magnetization, m(t), of the random transverse-field Ising chain after global quenches. We observe different relaxation behaviors for quenches starting from different initial states to the critical point. Starting from a fully ordered initial state, the relaxation is logarithmically slow and in a finite sample of length L the average magnetization saturates at a size-dependent plateau. Starting from a fully disordered initial state, the magnetization stays at zero for a period of time until $t=t_d$, which is exponentially large in l, l being the square root of L, and then starts to increase until it saturates to an L-dependent asymptotic value. For both quenching protocols, finite-size scaling is satisfied in terms of the scaled variable $\ln t/l$. Furthermore, the distribution of long-time limiting values of the magnetization shows that the typical and the average values scale differently and the average is governed by rare events. The non-equilibrium dynamical behavior of the magnetization is explained through semi-classical theory.

Critical behavior on complex networks: inhomogeneous mean-field vs Lee-Yang-Fisher formalism

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We study the critical behavior of spin models on a scale-free network with a power-law node-degree probability distribution decay $P(k) \sim k^{-\lambda}$, $k \gg 1$ and on a complete graph. To this end, we apply traditional inhomogeneous mean filed approach as well as we use the method of partition function zeros analysis in the complex temperature and magnetic field plane (Lee-Yang-Fisher formalism). The last method, to our knowledge, has not been used so far for scale-free networks.

For the Potts model on a scale-free network in terms of an inhomogeneous mean-field approach we find the set of critical amplitude ratios and scaling functions, which depend on the probability distribution decay exponent λ in the region $3 < \lambda < 5$. Moreover, we observe the non-typical behavior for the heat capacity jump δc_H [1]: for the Ising model on a scale-free network δc_H is λ -dependent even at $\lambda > 5$, while all critical exponents are λ -independent and correspond to the values predicted by the mean field theory.

We show that the angles that characterize partition function zeros location in the complex plane attain λ -dependence for $3 < \lambda < 5$ too. In particular, we derive the angle at which the Fisher zeros impact onto the real temperature axis. Our analysis of the Lee-Yang zeros reveals a difference in their behavior for the Ising model on a complete graph and on an annealed scale-free network. Whereas in the former case the zeros are purely imaginary, they have a non zero real part in the latter case, so that the celebrated Lee-Yang circle theorem is violated [2,3].

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Probing the energy landscape of neural networks

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Training neural networks with very low precision synapses has long been considered a challenging task even for the simplest neural architectures. In this talk I'll present a series of results which emerged from a large-deviation analysis using tools from Statistical Physics, which show that the training problem can be made algorithmically very simple by maximizing a "local entropy": explicitly seeking extensive regions in the space of configurations with low energy. Such regions also have some highly desirable properties, in particular very good generalization capabilities. These results appear to be rather general with respect to the details of the underlying model and of the data, and may be relevant biologically and technologically, as well as apply to other inference and constraint satisfaction problems.

[1] C. Baldassi, C. Borgs, J. Chayes, A. Ingrosso, C. Lucibello, L. Saglietti, and R. Zecchina. "Unreasonable effectiveness of learning neural networks: From accessible states and robust ensembles to basic algorithmic schemes", PNAS (2016)

Analytical results for the distribution of shortest path lengths in random networks

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The increasing interest in network research in recent years is motivated by the realization that a large variety of systems and processes which involve interacting objects can be described by network models. In these models, the objects are represented by nodes and the interactions are expressed by edges. The interactions between non-adjacent pairs of nodes are facilitated by paths going through intermediate nodes and edges. The shortest paths between such pairs are of particular importance because they provide the strongest interactions and fastest response. Therefore, the distribution of shortest path lengths (**DSPL**) is of great relevance to many dynamical processes taking place on networks such as diffusive processes, first passage processes, traffic flow, communication and epidemic spreading. We argue that the DSPL is a natural quantity by which dynamical processes on networks should be formulated. In particular, it incorporates the statistical symmetries of the network in the dynamical equations, in analogy to the reduction of a partial differential equation in Euclidean space to an ordinary differential equation for the radial component, in the presence of a spherical symmetry, and hence of fundamental importance.

While the average of the DSPL has been studied extensively, the analytical calculation of the entire distribution has remained an open problem. In this presentation a novel *analytical* approach for calculating the DSPL in random networks will be discussed. This approach is based on the cavity method, and applies to a large family of network types, which includes Erdos-Renyi networks [1], regular graphs and more generally, configuration model networks [2]. The results are found to be in agreement with numerical simulations for a broad range of networks, sizes and connectivities.

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Measuring effective temperatures in a generalized Gibbs ensemble

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The local physical properties of an isolated quantum statistical system in the stationary state reached long after a quench are generically described by the Gibbs ensemble, which involves only its Hamiltonian and the temperature as a parameter. If the system is instead integrable, additional quantities conserved by the dynamics intervene in the description of the stationary state. The resulting generalized Gibbs ensemble involves a number of temperature-like parameters, the determination of which is practically difficult. Here we argue that in a number of simple models these parameters can be effectively determined by using fluctuation-dissipation relationships between response and correlation functions of natural observables, quantities which are accessible in experiments.

Universal front propagation in the quantum Ising chain

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I will present recent results on the melting of domain walls in the ferromagnetic phase of the transverse Ising chain. The domain walls are created by flipping the order-parameter spins along one-half of the chain. If the flip is realized by a local operator in terms of Jordan-Wigner fermions, the resulting longitudinal magnetization profiles have a universal character. Namely, after proper rescalings, the profiles in the noncritical Ising chain become identical to those obtained for a critical free-fermion chain starting from a step-like initial state. The relation holds exactly in the entire ferromagnetic phase of the Ising chain. For the evolution of the entanglement entropy, we observe a saturation at the ground-state value for large times, suggesting a simple form of the steady state.

Many-body localization due to random interactions

Piotr Sierant ¹, Jakub Zakrzewski ¹, Dominique Delande ²

Many-body localized (MBL) systems, i.e. systems that do not thermally equilibrate under their own dynamics but rather evolve in such a way that the memory about local features of the initial state is preserved, have recently received a lot of attention. We consider a system of ultracold atoms in one-dimensional optical lattice with disordered on-site interparticle interactions. The MBL is found to occur in the system as one increases the interactions. The single-particle extended states are eigenstates in the absence of the disorder. Therefore, the observed localization is an inherent effect of the interactions and thus a genuine many-body effect. The localization is inspected by means of eigenvalue statistics as well as by time propagation of initial states with density wave order.

[1] arXiv:1607.00227, PRL submitted

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Dynamics of hybrid quantum systems

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The dynamics of a hybrid quantum system, composed by different subsystems, one of them being macroscopic, has been investigated in such a way to preserve genuine quantum effects even in the presence of a macroscopic part. The problem is related with the analysis of the quantum-to-classical crossover, but our approach allows us to take trace of the quantum correlations established between the microscopic and macroscopic components of the device. The specific systems we have considered model the macroscopic subsystem by one or more spin-S objects, with S large, and the actual calculation is made possible by a suitable approximation, valid in the large-S limit, which simplifies the spin-algebra. Two types of applications have been considered so far.

First, a quantum mechanical oscillator coupled to a spin environment has been considered, showing that an insightful expression for the propagator of the whole system can be found, where we can identify an effective "back-action" term, i.e. an operator acting on the magnetic environment only, and yet missing in the absence of the quantum principal system, which behaves as an effective time-dependent magnetic anisotropy, whose character, whether uniaxial or planar, also depends on the detuning between the frequency of the oscillator and the level-splitting in the spectrum of the free magnetic system, due to the possible presence of an external magnetic field.

The second system we considered is made by two qubits interacting with a spin-S chain, whose internal interactions allow for the propagation of soliton-like excitations. We have found that in the large-S limit the state of the chain can be sensibly described by coherent state products, so that the system dynamics while a soliton propagates through the chain can be numerically investigated. We have shown that in such hybrid devices, despite the large value of S, the spin chain can still act as a medium able to establish quantum correlations (entanglement) between two delicate, distant qubits, but at the same time its dynamical robustness, deriving from its non-linear macroscopic character, makes it possible to protect the qubits from the noisy effects of the outside world.

Non-Markovian quantum thermodynamics: second law and fluctuation theorems

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We bring together Keldysh theory and quantum thermodynamics, by showing that a real-time diagramatic technique can provide a quantum equivalent of stochastic thermodynamics for non-Markovian quantum machines (heat engines, refrigerators, etc). Taking any interacting quantum system with arbitrary coupling to ideal reservoirs of electrons and bosons (phonons or photons), we identify symmetries between quantum trajectories and their time-reverses on the Keldysh contour. These lead to quantum fluctuation theorems the same as the well-known classical ones (Jarzynski and Crooks equalities, non-equilibrium partition identity, etc), but which hold whether the system's dynamics are Markovian or not. Hence, such systems obey the second law of thermodynamics on average, even if fluctuations may violate it. Our proof applies to systems with Kondo effects or other strong correlations, and to systems in superposition states or with time-dependent driving.

[1] Preprint: arXiv:1611.00670

Crystallization of self-propelled hard-discs: a new scenario

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At low density, assemblies of self propelled particles are prone to a number of novel collective behaviors, which are specific to these intrinsically out-of-equilibrium systems. The high density phases of active matter have been much less studied. Either the density screens the activity and the liquid freezes according to equilibrium scenarii or activity dominates and new phases are prone to develop is an open question of major importance. Here we experimentally tackle this issue in the specific case of vibrated polar hard disks which are a model of self-propelled particle. We show that increasing density the quasi-continuous crystalization of equilibrium disks is replaced by a specifically active scenario. Clusters of dense hexagonallyordered packed discs spontaneously form, melt, split and merge leading to a highly intermittent and heterogeneous dynamics. No coarsening is observed. Increasing further the density, the clusters span a finite fraction of the system size and the structure becomes similar to that of a polycrystal. However the system is never frozen: the clusters permanently melt from place to place forming droplets of active liquid which rapidly propagate across the system. This state of affair remains up to the highest possible packing fraction questioning the stability of the crystal for active discs.

Odd viscosity in chiral active liquids

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Chiral active liquids, composed of self-rotating interacting units, are fluids that break both time reversal symmetry and parity. As a con- sequence, their viscous stress acquires an additional contribution called odd-viscosity (originally discovered in quantum Hall fluids) that is pro- portional to the angular momentum density. We construct a non-linear hydrodynamic theory of chiral active fluids, which captures previously neglected odd viscosity contributions. In the incompressible limit, the effect of odd viscosity is to modify the boundary pressure by an additional term proportional to the local vorticity. In the bulk, the odd viscosity affects the response of compressible chiral active fluids by gen- erating transverse currents (with respects to applied pressure) in Burgers shocks.

Statistical physics and melting Arctic sea ice

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Polar sea ice is a key player in the climate system and a critical indicator of climate change. For example, it reflects sunlight and helps mitigate solar heating of the Arctic Ocean. During late spring and summer, sea ice reflectance or albedo, a principal parameter in climate modeling, is largely determined by the evolution of surface melt ponds. As the ponds grow and coalesce, their fractal dimension undergoes a transition from 1 to about 2, around a critical length scale of 100 square meters in area. The ponds take on complex, self-similar shapes with boundaries resembling space-filling curves. I will discuss how methods from statistical physics, such as percolation, network and Ising models, are being used to quantitatively describe melt pond evolution and to address other multiscale problems in sea ice physics. Through our analysis of sea ice structures we have discovered an Anderson transition in disordered composite materials, where the eigenvalue statistics of a key random matrix governing classical transport transition toward universal Wigner-Dyson statistics as a percolation threshold is approached. Our work is helping to advance how sea ice is represented in climate models and to improve climate projections.

Large deviation theory applied to climate physics, a new frontier of statistical physics

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We propose to review some of the recent developments in the theoretical aspects of the non-equilibrium statistical mechanics of climate dynamics. At the intersection between statistical mechanics, turbulence, and geophysical fluid dynamics, this field is a wonderful new playground for theoretical physics involving tools from statistical physics: large deviation theory, path integrals, and diffusion Monte-Carlo algorithms. We will discuss two classes of applications. First extreme heat waves as an example of a rare events with huge impacts. Second rare trajectories that suddenly drive the complex turbulent dynamical system from one attractor to a completely different one, related to abrupt climate changes. Relation with instanton theory and effective models of first order transitions and their transition rates will be emphasized.

Memory and universality in interface growth

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In many physical systems, the interface of a stable phase growing into an unstable one exhibits, in presence of noise, a remarkably universal behavior, independent of the details of the growth mechanism: this is called the Kardar-Parisi-Zhang (KPZ) class of growth phenomena. Recent improvements in experimental protocols and theoretical methods led to major progress in understanding of this class, except for one important aspect: do statistical correlations survive during the time evolution? Here we provide a first analytical result, and a smoking gun experiment for it, which show how the memory of past growth is kept at later times in a quantitative manner. Our finding highlights persistent memory effects in non-equilibrium phenomena, which may also exist beyond the KPZ class.

[1] Jacopo De Nardis, Pierre Le Doussal, Kazumasa A. Takeuchi, arXiv:1611.04756

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Dynamical crossovers in prethermal critical states

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We study the prethermal dynamics of an interacting field theory with a N-component order parameter and O(N) symmetry, suddenly quenched in the vicinity of a dynamical critical point. Depending on the initial conditions, the evolution of the order parameter, as well as of response and correlation functions, can exhibit a temporal crossover between universal dynamical scaling regimes governed, respectively, by a quantum and a classical prethermal fixed point, as well as a crossover from Gaussian to prethermal dynamical scaling. Together with a recent experiment, this suggests that quenches can be used in order to explore the rich variety of dynamical critical points occurring in the non-equilibrium dynamics of a quantum many-body system. We illustrate this fact by using a combination of functional renormalization group techniques and a non-perturbative large-N limit.

A statistical physics approach for the flow transition of yield stress fluids

Kirsten Martens

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In this talk I will discuss several mesoscopic approaches, such as lattice models [1] and mean-field descriptions [2] for the yielding transition and the non-linear rheology of driven yield-stress materials. Despite the fact that this type of models require some phenomenological ingredients, notably the detailed local yielding rules, they have been shown to match several aspects of the mechanical response very well, such as avalanche statistics [1], mechanical noise descriptions [3] and rheological features, like for example shear banding [4] and creep dynamics. Further the mesoscopic approach provides an ideal tool to test basic assumptions for different flow phenomena and can serve as a bridge to large scale descriptions of the complex yielding dynamics.

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Hysteresis in the random-field Ising mode

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The random-field Ising model (RFIM) is one of the simplest statistical-mechanical models that captures the anomalous irreversible collective response seen in a wide range of physical, biological, or socioeconomic situations in the presence of interactions and intrinsic heterogeneity or disorder. When slowly driven at zero temperature, it can display an out-of-equilibrium phase transition associated with critical scaling ("crackling noise"), while it undergoes at equilibrium, under either temperature or disorder-strength changes, a thermodynamic phase transition. Phase transitions in RFIM are characterized by a huge number of quasidegenrate metastable states. To fully capture the important physics we have used the Nonperturbative Renormalization Group (NPRG) approach. I will present our recent understanding of the hysteresis phase transition. We show that the fixed point describing hysteresis is different from the fixed point describing the equilibrium phase transition, despite several surprising indications that the two transitions were governed by the same fixed point. Our starting point is a dynamical formalism that we developed within the NPRG.

Sherrigton-Kirkpatrick glassy-phase of random Josephson coupled Bose-Einstein condensates in wood-pile geometry

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We study a transition to a glassy phase of neutral atoms trapped in optical lattice, where the system is realized as the array of individual Bose–Einstein condensates of N elongated vertical and horizontal N rods in a wood-pile form coupled via the random Josephson tunneling. In this geometry every horizontal (vertical) rod of a condensate is linked to its vertical (horizontal) counterpart, so that the number of nearest neighbors z of a given rod in this system is z=N, implying that the system is fully connected. This together with randomness forms a prerequisite of the Sherrington-Kirkpatrick model for infinite N widely employed in the theory of spin glasses. For this arrangement we solve a model Hamiltonian of the Josephson array in the thermodynamic limit and calculate the critical temperature for the glassy phase-locking transition, caused by the Josephson tunneling of bosons in random environment.

Quantum Kasteleyn transition

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Dimer models arise as effective descriptions in a variety of physical contexts, and provide paradigmatic examples of systems subject to strong local constraints. Their classical statistical mechanics can be understood in terms of a continuum height model (in 2D) or gauge theory (in 3D), and exhibits unusual phenomena such as algebraic correlations and deconfinement of monomer excitations. In this talk, I will present the quantum version of the venerable Kasteleyn model, which has an unusual phase transition from a dimer solid to a U(1) liquid, and show how the phase structure can be understood in terms of the quantum mechanics of one-dimensional strings. The model provides new insights into the physics of U(1) quantum spin liquids, shedding light on the Polyakov argument for their absence in 2D, and, in 3D, providing a tractable limit for calculation of their properties.

Simulating condensed matter with ultracold atoms: the Haldane model and the Peierls substitution

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The Haldane model is a celebrated two-dimensional tight-binding model characterized by a quantum Hall effect due to the breaking of time-reversal symmetry, with zero net magnetic flux through the unit cell [1]. It is characterized by exotic quantum phases with different Chern numbers, depending on the value of the phase of the next-to-nearest tunneling amplitude. In its original formulation [1], the model is constructed by means of the so-called Peierls substitution (PS) [2,3], a popular approach that is widely employed in the literature to account for the effect of a vector gauge field A in the tight-binding description of electrons, as well as for ultracold atoms in optical lattices in the presence of artificial gauge fields. In the tight-binding language, it amounts to adding to the "bare" tunneling coefficients a phase factor proportional to the line integral of A. Despite its popularity, the PS is a rather uncontrolled approximation. Though this has been remarked from time to time in the literature [6,7], the general tendency is to use the PS as a sort of minimal coupling for tight-binding models, and this can lead to severe failures.

In a recent work [8], we have pointed out that the conditions for the applicability of the PS are explicitly violated in the Haldane model and in any other model where the vector potential varies on the same scale of the underlying lattice. Nonetheless, we have shown that the general structure of the Haldane model is in fact preserved, as it is a direct consequence of the symmetries of the system, and no additional assumptions are required. In addition, we have shown that the values of the tunneling coefficients can be obtained from simple closed expressions in terms of gauge invariant, measurable properties of the spectrum (namely, the gap at the Dirac point and the bandwidths). These formulas evidence that the phase acquired by the next-to-nearest tunneling amplitude is quantitatively different from that predicted by the PS, and it also presents a pronounced dependence on the intensity of the underlying lattice potential. Moreover, even the tunneling amplitudes turn out to be dependent on the intensity of A, violating the hypotheses behind the PS. These results have been also checked against ab-initio calculations by means of the maximally localized Wannier functions (MLWFs) [9], which are also helpful in understanding the origin of the breakdown of the PS.

I will present a pedagogical introduction to the Peierls substitution, the role of the MLWFs in the construction of tight-binding models for ultracold atoms in optical lattices, and their implications in the derivation of the Haldane model.

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Contributed Poster Presentations

Soft matter and biophysics

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2 Beelen Charlotte, Hartmann Alexander

Large Deviation Properties of RNA Neutral Set Size

3 Hobrecht Hendrik, Hucht Fred

Testing conformal invariance in near-critical colloidal suspensions

4 Lopes Cardozo David, Holdsworth Peter, Ciliberto Sergio, Puosi Francesco

Direct calculation of the critical Casimir force by simulation of a binary fluid

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Granular gas experiments to investigate Non-Equilibrium Steady States

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Phases and colloidal quasicrystals of lipid A-phosphate structures

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Multiple hysteresis behaviors in spin models

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Annex: Abstracts of Poster Presentations

Scalings, saddle points and Gaussian variational method revisited for the 1D interface in random media

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We discuss as a case study the scaling properties of a one-dimensional interface at equilibrium, at finite temperature and in a disordered environment with a finite disorder correlation length. We focus our approach on the scalings of its geometrical fluctuations, specifically of the variance of its relative displacements at a given length scale. This 'roughness' follows at large length scales a power law whose exponent characterises a superdiffusive behaviour, which in 1+1 dimension is known to be the characteristic 2/3 exponent of the Kardar-Parisi-Zhang (KPZ) universality class. On the other hand, the Flory exponent of this model, obtained by a power counting argument on the interface Hamiltonian, is equal to 3/5 and thus does not yield the correct KPZ roughness exponent. However, a standard Gaussian-Variational-Method (GVM) computation of the roughness is supposedly bound to predict the Flory exponent instead of the physical KPZ one.

In this work, we first review some of the available power-counting options, and examine the distinct exponent values that they predict. Their (in)validity is shown to depend on the existence (or not) of well-defined optimal trajectories in a large-size or low-temperature asymptotics. We identify the crucial role of the 'cut-off' lengths of the model-the disorder correlation length and the system size - which one has to carefully follow throughout the scaling analysis. In particular, we report new results obtained within a GVM computation scheme which

includes explicitly a finite system size, allowing to avoid the usual Flory pitfall and thus to predict correctly a 2/3 asymptotic roughness exponent.

<u>Reference</u>: Elisabeth Agoritsas and Vivien Lecomte, arXiv:1610.01629 [cond-mat.stat-mech], " Power countings versus physical scalings in disordered elastic systems - Case study of the one-dimensional interface"

Multiple hysteresis behaviors in spin models

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Hysteresis is simply defined as history dependent variation of the magnetization with magnetic field, and it is one of the important properties of magnetic materials. Multiple hysteresis behaviors may appear in some physical systems such as Fe3O4 / Mn3O3 superlattices [2] and molecular based magnetic materials [2]. Theoretically, it was shown that some spin models in different geometries could exhibit multiple hysteresis behaviors, e.g. magnetic nanowires [3].

Recently, it has been observed that S-1 Anisotropic Heisenberg model could display double hysteresis behavior [4]. In the isotropic Heisenberg limit, this behavior was never observed while the highly anisotropic limit (i.e. Ising model) has double hysteresis behavior [5]. Then, several question about the multiple hysteresis behaviors in other spin models may arise such that "Can the higher spin models exhibit multiple hysteresis behaviors?" or "What is the effect of quenched disorder on these type phenomena?" Hence, the aim of this talk is to present the results obtained regarding the higher spin models within the effective field theory, which is one of the most widely used methods in statistical physics of magnetism. Besides, the effect of the disorder on these hysteresis behaviors will also be discussed.

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Breakdown of the Bose-Einstein condensation induced by long-range interactions within the Hartree-Fock approximation

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We consider a Bose gas with two-body interactions $V(r) = \gamma^3 v(\gamma r)$ where v(x) is a given repulsive and integrable potential, while γ is a positive parameter which controls the range of the interactions and their amplitude at a given distance. Previously, within the Kac scaling, it has been proved in the literature that, in the limit $\gamma \to 0$, the gas still undergoes a Bose-Einstein condensation. This can be easily understood by noticing that for $\gamma = 0$, the particles feel a uniform potential which only shifts their kinetic energies by the constant $a\rho$, where ρ is the particle density and a is the fixed spatial integral of V(r). For non-zero values of gamma, that simple picture is no longer valid and the existence of a condensate is questionable. In fact, using the Hartree-Fock approximation, we find that the condensate is destroyed by the repulsive interactions when they are sufficiently long-ranged. More precisely, we show that, for gamma sufficiently small but finite, the off-diagonal part of the one-body density matrix always vanishes at large distances. Our analysis sheds light on the coupling between critical correlations and long-range interactions, which might lead to the breakdown of off-diagonal long-range order. The exact status of that breakdown beyond the Hartree-Fock approximation itself remains an open question.

MECO42

Entanglement and thermodynamics after a quantum quench in integrable systems

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Entanglement and entropy are key concepts standing at the foundations of quantum and statistical mechanics, respectively. In the last decade the study of quantum quenches revealed that these two concepts are intricately intertwined. Although the unitary time evolution ensuing from a pure initial state maintains the system globally at zero entropy, at long time after the quench local properties are captured by an appropriate statistical ensemble with non zero thermodynamic entropy, which can be interpreted as the entanglement accumulated during the dynamics. Therefore, understanding the post-quench entanglement evolution unveils how thermodynamics emerges in isolated quantum systems. An exact computation of the entanglement dynamics has been provided only for non-interacting systems, and it was believed to be unfeasible for genuinely interacting models. Conversely, here we show that the standard quasiparticle picture of the entanglement evolution, complemented with integrability-based knowledge of the asymptotic state, leads to a complete analytical understanding of the entanglement dynamics in the space-time scaling limit. Our framework requires only knowledge about the steady state, and the velocities of the low-lying excitations around it. We provide a thorough check of our result focusing on the spin-1/2 Heisenberg XXZ chain, and considering quenches from several initial states. We compare our results with numerical simulations using both tDMRG and iTEBD, finding always perfect agreement.

Unveiling a critical point in glasses through high order non-linear measurements

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Although structural glasses are everyday materials playing an increasing role in modern technological applications [1], the glass transition in itself remains a conundrum. Over the two past decades several experimental breakthroughs have deepened our understanding of glasses. Among them, the developpement of third order nonlinear response measurements [3,4,5,6,7] have been instrumental in putting forward new ways of measuring a significantly non-trivial thermodynamic response.

This talk will be devoted to showing how fifth order non-linear responses allows us to infer very strong experimental indications of the existence of a thermodynamic critical point in several archetypical glass formers [2]. Time permitting, various kinds of experimental nonlinear responses will be compared [3,4,5,6,7] with these results, aiming at giving a unified physical picture of the non-linear response in dielectric glass formers.

We thank C. Alba-Simionesco, A. Coniglio, P.-M. Déjardin, G. Tarjus, and M. Tarzia for interesting discussions. The work presented here was supported by ERC grant NPRGLASS, by the Labex RTRA grant Aricover, by the Institut des Systèmes Complexes ISC-PIF and by the Deutsche Forschungsgemeinschaft via Research Unit FOR1394.

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Superglass phase of interaction-blockaded gases on a triangular lattice

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Much effort has been devoted to the study of glassy phases for lattice systems, and in particular to the coexistence of glassiness behaviour with quantum effects, like Superfluidity or Bose-Einstein Condensation. These superglass phases have been observed in continuous space systems and in lattice models, but up to now their experimental realization remains inconclusive.

We investigate the quantum phases of monodispersed bosonic gases confined to a triangular lattice and interacting via a class of soft-shoulder potentials. Using exact quantum Monte Carlo simulations, we determine the equilibrium phases of the model to be a superfluid, a supersolid, and a crystal for increasing interaction strength. Quenching in temperature results in the appearance of a glass and a superglass region, for strong and intermediate values of the interaction strength, respectively. These glass phases are obtained in the absence of externally induced frustration in the model (usually employed to generate glassy behaviour) and, in the case of the superglass phase, glass physics coexists with a sizable superfluid fraction. The interactions we choose to simulate are relevant for experiments with Rydberg-dressed atoms in optical lattices, and therefore these phases should be possible to observe in state-of-the-art experimental setups.

STRUCTURAL AND DYNAMIC FEATURES OF IONIC LIQUIDS SOLUTIONS WITH AROMATIC HYDROCARBONS

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Ionic liquids (ILs) have been extensively studied as replacements to sulfolane in the separation of aromatics from alkanes. The employment of ILs could reduce energy requirements and operating costs of the aromatic extraction unit as a result of their nonvolatile character. However, the ILs studied so far have shown mass-based aromatic distribution ratios lower than the sulfolane values, which would increase the solvent-to-feed ratio in the extractor. The performance of hydrophobic ionic liquid (dimethyl-imidazolium chloride) on extraction of aromatic compounds such as benzene, toluene, anisole, phenol and c-hexane derivatives from aqueous solution was investigated experimentally.

The MD method was applied using a modified DL_POLY_4.05 with a time step of 2 fs. The long-range electrostatic interaction was taken into account by the Ewald method. In the calculations, the cations, anions, and atoms forming the molecules of the added substance (hydrocarbons: benzene, toluene, phenol, anisole and c-hexane) ware treated as solid charged model systems with a fixed geometry. The methyl in the dmim+ and toluene ware treated as a pseudoatom with the total charge. All the studies were conducted for systems composed of 192 dmim+ cations, 192 chlorine anions Cl-, and one solute molecule at T = 400 K. The unit cell volume was calculated from the experimental values of the ionic liquid density at T = 400 K. The calculations used periodic boundary conditions. The electrostatic interaction at short distances was described using point charges on each atom. The interaction between dm?m+ and Cl- molecules in the ionic liquid was described using the Buckingham potential for inter-

actions at short distances. The Berendsen thermostat was used to stabilize the system in the $N\ V\ T$ -ensemble.

Analysis of the data allowed to establish: (1) The salvation effect in systems ionic-liquid (dmim+/Cl-) - non-polar solute molecules (benzene, c-hexane) has qualitatively similar to the behavior of the hydrophobic hydration of aromatic solute molecules in liquids like water. The results of the computer experiment for the average total energy of the intermolecular interaction < Etot> for the dmim+/Clnon-polar solutions at T = 400 K show that the intermolecular interaction < Etot> does not depend on the physical characteristics of the structural and non-polar substances dissolved. Therefore, as a possible selection criteria for the data analysis is not appropriate to consider the thermodynamic and structural characteristics of the system. In this case, need to do analysis of its dynamic properties. Based on the data obtained from MSD and VAF the different diffusion mechanisms of nonpolar solute molecules in IL ware determined. (2) The salvation effect in systems ionic-liquid (dmim+/Cl-) - polar solute molecules (toluene, phenol, anisole) has qualitatively similar to the behavior of the hydrophobic hydration in liquids like water too. The results of the computer experiment for the average total energy of the intermolecular interaction < Etot> for the dmim+/Cl-polar hydrocarbons at T = 400 K show that the intermolecular interaction < Etot> depend on polarity and the physical characteristics of the structural and polar substances dissolved. Based on the data obtained from MSD and VAF the different diffusion mechanisms of polar hydrocarbons solute molecules in IL ware determined. (3) Dissolution of hydrocarbons molecules whose size is much higher than the maximum length of the hydrogen bond leads to a radical restructuring of the network of hydrogen bonds in the system up to the loss of its percolation properties.

The results showed that IL had good ability in the extraction. Molecular structure of aromatic compounds was found to have a great influence on the extraction. Due to the increase of the hydrophobicity of solute, the partition coefficient of aromatic compounds was increased.

Phase diagram of a two dimensional electron glass

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We investigate the phase transition in two dimensional electron glass, which is a system in which all the electron states are localised. We model the system by a square lattice of localised states which have random energies and interact via long-range Coulomb potential. Further a much discussed question is whether there is an equilibrium transition to glassy phase or a charge ordered phase as the temperature is lowered and disorder is increased. For a three dimensional Coulomb glass Martin Goethe have found a transition from charge ordered phase to paramagnetic phase for small disorders and no evidence of glass transition at higher disorders. We have used Monte Carlo annealing to study the system where only half the sites are occupied and the number of particles are conserved. We found a charge-ordered phase whose transition to fluid phase is of secondorder type at very weak disorder strength, where the transition temperature was calculated using the finite size scaling. In the higher disorder regime the hysteresis studies show a transition from ordered phase characterized by large clusters (no long range order exists) to a paramagnetic phase. We did not find evidence of glassy phase at any finite temperature and disorder strength.

Large Deviation Properties of RNA Neutral Set Size

Charlotte Beelen ¹, Alexander Hartmann ¹

The functionality of noncoding RNA molecules is mainly determined by their structure. Sequences with the same structure form the *neutral set*. The neutral set may be partitioned into several components, called neutral networks, traversable by structure-preserving point mutations. The neutral network size is biologically relevant: large neutral networks appear to be favourable in terms of mutational robustness and evolvability. We investigate the neutral set and neutral network size using computer simulations.

We apply a dynamic programming approach [1] to obtain the secondary structures of RNA sequences. The neutral set size can be estimated using a *Nested Set Monte Carlo* Simulation [2]. We implemented a combination of the algorithm with the *Ballistic Search* approach to estimate the neutral network size. The distribution of neutral set and network sizes is determined for randomly generated RNA and compared to biological RNA molecules. To improve the accuracy in the tails of the distribution, large-deviation simulations are used [3]. Furthermore, the correlation of the neutral set size to other observables like the number of base-pairs is investigated.

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The quest for the missing noise in a micro-mechanical system out of equilibrium

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Equipartition principle plays a central role in the understanding of the physics of systems in equilibrium: the mean potential and kinetic energy of each degree of freedom equilibrates to kT/2, with k the Boltzmann constant and T the temperature. This equality is linked to the fluctuation-dissipation theorem (FDT): fluctuations of one observable are proportional to the temperature and dissipation in the response function associated to that observable. In non equilibrium situations however, such relations between fluctuations and response are not granted, and excess noise is usually expected to be observed with respect to an equilibrium state.

In this presentation, we show that the opposite phenomenon can also be experimentally observed: a system that fluctuates less than what would be expected from equilibrium! Indeed, when we measure the thermal noise of the deflexion of a micro-cantilever subject to a strong stationary temperature gradient (and thus heat flow), fluctuations are much smaller that those expected from the system mean temperature.

We will first present the experimental system, an atomic force microscope (AFM) micro-cantilever in vacuum heated at its free extremity with a laser. We will show that this system is small enough to have discrete degrees of freedom but large enough to be in a non-equilibrium steady state (NESS). We will then estimate its temper-

ature profile with the mechanical response of the system [1], and observe that equipartition theorem can not be applied for this NESS: the thermal noise of the system is roughly unchanged while its temperature rises by several hundred degrees! We will explain how a generalized FDT taking into account the temperature field can account for these observations, if dissipation is not uniform. Further experimental evidences of the validity of this framework will conclude the presentation.

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Resonant fluorescence in a monochromatically driven two-level quantum system with broken inversion symmetry

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Resonant fluorescence phenomenon in a two-level quantum system possessing dipole moment operator with permanent non-equal diagonal matrix elements and driven by an external semi-classical monochromatic EM (laser) field was studied. An expression for the fluorescent radiation spectrum in a far-distant zone was derived. It was shown that such two-level system can radiate continuously at much lower frequency when driven by high-frequency laser field. It was also found that the same driven two-level quantum system is able to amplify weak probe EM radiation waves belonging to the low frequency range. Possible ways to observe the predicted effects experimentally and employ them for a wide range of practical applications are discussed.

The investigation of the lateral interaction in cellular automaton traffic flow model with open boundaries

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Traffic flow models based on periodic boundaries have been intensively studied before. However, the traffic behavior under open boundaries has played an important role in statistical mechanics. Indeed, traffic flow shows phase transition which is induced by the boundaries. Such transitions have no counterpart in the one dimensional equilibrium systems. This fact has led many physicists to address open systems using different strategies of injections. The extension of the different traffic phases for open boundaries depends on the adopted injection strategy of vehicles [1-3]. In this context, we proposed a new injection strategy in which a reentrance phenomenon appears with an extension of the low density phase [3]. In the deterministic case, the reentrance is exhibited for high injection rate. However, for the non-deterministic case, the reentrance shifts to higher values of extraction rate. The main mechanism that induces that phenomenon is the inflow function. Indeed, by adopting our injection rule, the injection rate and the inflow are not equal. Furthermore, an injection rate exists, above which the in-flow begins to decrease by increasing the injection rate.

In the previous work [3], only longitudinal interactions between vehicles are taken into account. In fact, vehicles may interact laterally in many situations. This kind of interaction is noticeable in real traffic flow and was studied by using the periodic boundaries [4]. However,

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the traffic behavior with an open system is not taken into account. This fact have led us to investigate analytically and by numerical simulations the effect of defects on the phase diagram by using our new injection strategy [3]. Indeed, we have found that the presence of defects induces a lateral interaction between the defects and vehicles [4]. In this work, we have found that with the presence of defects (impurities), the inflow function depends on the defects permeability (the probability of lateral deceleration [4]) and their distribution on the lattice. In that respect, two cases were studied: the random distribution of defects and the compact distribution of defects. It is found that the random distribution of defects reduces the inflow. Subsequently, the low density phase region expands. However, for a compact distribution of defects, the inflow keeps unchanged which induces an expansion of the high-density phase with a maximum current phase appearance. In this context, the maximum current phase is studied in sufficient detail to explain his apparition by considering the lattice inflow and the defects region inflow.

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Work, work fluctuations, and free energy from kinetic theory

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The Boltzman-Loretnz kinetic equation (1) describes the dynamics of a particle immerse in a low density gas at equilibrium, and there is no doubt about its

validity in the appropriate limit. Since it does not contain any hypothesis about the macroscopic description of the state of the particle, it seems an appropriate starting point to investigate questions related with the thermodynamic description of a particle in contact with a heat bath and, in particular, the validity under those circumstances of the two work theorems proposed by Jarzynski (2) and by Bochkov and Kuzovlev (3), respectively. It must be realized that these theorems are derived using reversible hamiltonian dynamics. Moreover, both theorems use different definitions of work, and the question of the relevance of both definitions in the context of thermodynamic is addressed. The theoretical analysis is complemented by particle simulations of the Boltzmann-Lorentz equation using the Direct Simulation Monte Carlo (DSMC) method. The conclusion reached is that the Jarzynski definition of work seems more appropriate for inhomogeneous systems, but that this theorem is not suitable when the dynamics of the macroscopic system, i.e. the time interval in which the measurements are carried out, occurs on time scales over which relaxation to equilibrium is observed. On the other hand, the theorem by Bochkov and Kuzovlev, referring to the usual thermodynamical definition of work for homogeneous systems, seems to be obeyed also when the tendency to the steady state must be taken into account.

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The modified Poisson-Boltzmann equation: Explicit account of the polarizable co-solvent

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The Poisson-Boltzmann (PB) equation remains the simplest and very efficient tool for describing distribution of charged particles near the macroscopic charged surfaces in many areas, such as biophysics, electrochemistry, chemical engineering, etc [1]. As is well known, the PB equation is based on the mean-field theory that makes its application to the real systems quite problematic. Firstly, the mean-field theory itself does not allow us to take into account the effects of the ionic correlations that are crucial for concentrated enough electrolyte solutions. Secondly, considering the solvent as a continuous dielectric medium makes it impossible to study the effects of the solvent molecular structure. These two reasons have motivated the researchers to improve the PB equation in the last two decades [2]. In present report a theoretical research [3,4] on the effects of the polarizable co-solvent in the electric double layer theory will be presented. The derivation of the modified PB equation with explicit account of the polarizable co-solvent molecules within both the field-theoretical formalism and density functional theory will be demonstrated. An influence of the co-solvent polarizability in combination with the excluded volume of the co-solvent molecules on the differential capacitance of electric double layer will be discussed.

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Anisotropic domain growth in the d=3 Ising model with dipolar interactions

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Our work focuses on dipolar systems which are ubiquitous, but have received limited theoretical attention. Some examples include alkali hydrides, rare earth fluorides and chlorides, uniaxial ferroelectrics, etc. They are well-represented by the Ising model with dipolar interactions (IM+DI). The latter are long-ranged, anisotropic and can be positive or negative depending on the relative positions of the interacting dipoles. Equilibrium studies have revealed novel consequences of these complicated interactions, but their effect on nonequilibrium aspects is unexplored. We perform, for the first time, a deep temperature quench to study the kinetics of domain growth in IM+DI. Our main observations are: (i) Emergence of elongated domains along the z-axis (Ising axis) with a signature of periodicity in their arrangement in the xy-plane; (ii) Anisotropic domain growth laws with distinct power law exponents in the z-direction and perpendicular to it; (iii) Presence of generalized dynamical scaling signifying that in domain growth the dipolar strength is relevant only upto a scale factor; (iv) Smooth interfaces, as characterised by the Porod law, inspite of the competing ferromagnetic and antiferromagnetic interactions. These observations are relevant for the wide range of experimental systems represented by IM+DI.

Applications of maximal entropy random walk

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The concept of maximal entropy random walk (MERW) is based on the idea of equiprobable trajectories (Phys. Rev. Lett. 102, 160602). The most surprising feature of this type of random walk is that it exhibits localisation on almost regular lattices with a weak disorder coming from diluted irregularities of the lattice. In the talk we shortly recall the definition of MERW and discuss its various applications.

Storage properties and hard-spheres packing in perceptron and support vector machines

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The goal of the project is to provide a theoretical analysis of the properties of two different models, which are usually used as supervised learning algorithms: perceptron and support vector machines. From an abstract point of view these models can be interpreted as constraint satisfaction problems, which show a SAT-UNSAT phase transition at thermodynamical limit. In this framework the so-called storage problem for perceptron is found to be equivalent to a hard sphere-packing problem. The first part of the work focuses on the storage properties of a slighly modified version of the perceptron, in which one parameter is considered as a random variable. The second part is a starting point to approach the same kind of problem in support vector machines and to point out some possible source of error present in already known results. The whole work is carried out through statistical physics methods and tools used to study disordered systems - such as spin glasses - whose main ingredient is the famous replica method.

First passage fluctuation relations rules by cycle affinities

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For a non-equilibrium stationary state described by a Markovian process it is well known that the entropy production rate can be expressed in terms of the affinity associated with every transition in the graph representation of the master equation. We exhibit the invariance of cycle affinities in finite state Markov processes under various natural probabilistic constructions: for instance under conditioning and under a new combinatorial construction that we call "drag and drop". For semi-markovian processes whose corresponding graph is made of a single cycle, we establish that the cycle current obeys a fluctuation relation for first passage times at integer winding numbers, which is dual to the fluctuation relation for the cycle current at fixed time: contrarily to seminal fluctuation relations about the probabilities for measuring a random cumulative exchange quantity or its opposite value during a given time, the latter fluctuation relations deal with the probabilities for the random time needed for one cycle to be performed in one sense or in the opposite one with a given winding number.

Reference: M. Bauer and F. Cornu, J. Stat. Phys. 155 (2014) 703-736.

Dielectric Spectroscopy of a Stretched Polymer Glass: Heterogeneous Dynamics and Plasticity

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We study the dielectric relaxation of polycarbonate (PC) at room temperature under imposed strain rate γ , above the yield stress, and up to 13% strain. We find that the dielectric response of stretched PC behaves as if it was heated up at a temperature just below its glass transition temperature, T_g around 423 K for PC. Indeed, in the frequency range of our experiment (10^{-2} and 10^3 Hz), the dielectric response of the stretched PC at room temperature superimposes to the dielectric response of PC at a temperature $T_a(\dot{\gamma}) \leq T_g$, which is a function of strain rate. Specifically we observe that at T_a the dominant relaxation time $\tau_\alpha(T_a)$ of PC at rest is related to $\dot{\gamma}$ in such a way that $\tau_\alpha(T_a) \sim 1/\dot{\gamma}$ at and beyond the yield point. In our experiment, $10^{-5}s^{-1} < \dot{\gamma} < 10^{-3}s^{-1}$, the temperature shifts $T_g - T_a$ are of a few kelvin. The mechanical rejuvenation modifies the dielectric response at frequencies smaller than 10 Hz, whereas for higher frequencies the spectrum is only slightly modified.

Universal correlations of the one-dimensional delta Bose gas in a non-uniform trapping potential

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Many large-scale, universal, effects in one-dimensional systems at quantum critical points can be tackled with a combination of methods from solvable lattice models and from field theory, usually conformal field theory (CFT) and Luttinger liquid ideas. Yet, the applicability of such tools in condensed matter physics is often limited to situations in which the bulk is uniform: CFT, in particular, describes low-energy excitations around some energy scale, assumed to be constant throughout the system. However, in many experimental contexts, such as quantum gases in trapping potentials and in many out-of-equilibrium situations, systems are strongly inhomogeneous. We will argue that standard CFT methods can nevertheless be extended to deal with such 1D situations, and we will illustrate the main idea with the example of the delta Bose gas. The method we develop can be thought of as the Local Density Approximation (LDA) on steroids: while standard LDA allows to calculate density profiles (more generally, expectation values of local operators), here we use LDA to extract the position-dependent parameters that enter the field theory action, such as the components of the metric tensor. Then, once the action has been fixed, all correlation functions follow: this strategy will be illustrated with new results about entanglement entropies in trapped one-dimensional gases.

Finite Temperature Magnetic Properties of the Quenched Disordered Binary Alloy Nanowire: A Monte-Carlo Simulation Study

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Finite temperature magnetic phase transition properties of a ferromagnetic binary alloy nanowire have been investigated by means of Monte Carlo method based on local spin update Metropolis algorithm. The magnetic components *A* with spin-1/2 and *B* with spin-1 are distributed randomly throughout the nanowire with a probability of p and 1-p, respectively. Our simulation results indicate that the phase boundary lines, magnetization profiles and magnetic susceptibility behaviors of the nanowire are sensitively depend on the values of concentration of the type-A magnetic components, the exchange interaction strengths between randomly located atoms and also single ion anisotropy term.

Triple-parabola approximation for interfacial properties of binary mixtures of Bose-Einstein condensates

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Accurate and useful analytic approximations are developed for order parameter profiles and interfacial tensions of phase-separated binary mixtures of Bose-Einstein condensates with repulsive interatomic forces. A triple-parabola approximation (TPA) is proposed, to represent closely the energy density featured in Gross-Pitaevskii (GP) theory. This TPA allows us to define a model, which is a handy alternative to full GP theory, while still possessing a simple analytic solution. The TPA offers an improvement over the recently introduced double-parabola approximation (DPA). In particular, a more accurate amplitude for the wall energy (of a single condensate) is derived and a more precise expression for the interfacial tension (of two condensates) is obtained, while also the interface profiles undergo a qualitative improvement [1].

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Langevin equations for reaction-diffusion processes

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Langevin equations are ubiquitous in the modelization of out-ofequilibrium systems and provide a starting point both for numerical simulations and field theory approaches. Most of the time, these equations are derived in a phenomenological way by adding a noise term - which is supposed to modelize the complicated microscopic degrees of freedom of the system - to a deterministic mean-field equation. However, I will show in my presentation that it is possible for some systems (the reaction-diffusion processes) to start from the microscopic dynamics and, without any approximation, to obtain a Langevin equation that describes the system exactly (Benitez, Duclut et al., PRL 2016). Obviously, this exact description of the system by a Langevin equation has a cost: The Langevin equation is not stated in terms of a "physical" variable but rather in terms of an "auxiliary" variable. I will however show that with the help of a duality relation, all the physics can be extracted from this auxiliary variable (Doering, Mueller, Smereka, Physica A 2003).

Since these Langevin equations are exact (and real) – in particular in the low density regions – they are the right starting point for numerical and theoretical studies of reaction-diffusion processes (Dornic, Chaté, Muñoz, PRL 2005).

Cooperativity and laning of driven tracers

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Several tracers driven in a dense bath tend to follow each other to increase their mobility, thereby forming lanes. This phenomenon is encountered in suspensions of charged colloids as well as in pedestrian traffic. The nature of this so-called "laning transition" has been debated: is it a crossover or a phase transition? In order to quantify the order in the system, we focus on the correlations between the tracers themselves and between the tracers and the bath. Our analytical approach is based on the linearization of the stochastic equations for the density fields. The correlations are found to be anisotropic and long ranged. Brownian dynamics simulations confirm our results and show that the shape that we predict holds far beyond the validity range of our computation, suggesting that it is universal. Finally, I discuss the model dependence of this behavior.

Dynamic quadrupolar susceptibility for the spin-1 Blume-Emery-Griffiths model

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The spin-1 Blume-Emery-Griffiths (BEG) model [1] is a spin system which contains biquadratic exchange interactions (K) and the crystal field (D) (or quadrupolar field) in addition to bilinear exchange interactions (J). Recently, the linear response of the quadrupolar order parameter to the crystal field which is also known as the static quadrupolar susceptibility for the BEG model has been studied within mean-field approximation by us [2]. In this work, the dynamic response of the same spin system in the presence of a periodically varying time-dependent crystal field is formulated on the basis of Onsager theory of irreversible thermodynamics. An expression for the dynamic (or complex) quadrupolar susceptibility is calculated. From the real and imaginary parts of this expression, dispersion relation and absorption factor for the quadrupolar field are derived. The temperature and crystal field variations of these quantities for both lowand high-frequency regimes are analyzed using two different phase diagram topologies which take place for K/J=3.0 and K/J=5.0. In particular, their behaviours for temperatures and crystal field values less than, equal to, and greater than the second-order phase transition are investigated. From this investigation frequency dependent peaks (or maxima) are observed in the ordered and disordered phases. We also show that by definition the quadrupolar dispersion converges to the corresponding static quadrupolar susceptibility in the zero frequency limit [2].

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Non-local orders and exotic phases in Hubbard-like low dimensional systems

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The experimental realization of time-dependent ultracold lattice systems has paved the way towards the implementation of new Hubbard-like Hamiltonians. We show that in a one-dimensional twocomponent lattice dipolar Fermi gas the competition between long range repulsion and correlated hopping induced by periodically modulated on-site interaction allows for the formation of hidden magnetic phases, with degenerate protected edge modes. The magnetism, characterized solely by string-like nonlocal order parameters, manifests in the charge and/or in the spin degrees of freedom [1]. In the spin sector, the underlying order is associated with the presence of a delocalized alternation of up and down spins in a background of doublons and holons (where a doublon consists of two fermions with opposite spin on the same lattice site and an holon is an empty site). In the charge sector the role of the up and down spins and that of doublons and holons is reversed; thus the magnetism consists in the presence of alternated and diluted doublons and holons in a string of singly occupied sites. Phases associated with the parity order, where holons and doublons or up and down spins appear to be localized in pairs, are also present in the phase diagram of our model. We also discuss to which extent non-local orders can characterize the physics of higher dimensional interacting quantum systems, and whether string order parameters are still suitable, upon appropriate generalization, for capturing it. We present the generalization of the definition of the parity operators to the two dimensional case [2] and apply it to study the superfluid-Mott insulator transition in the Bose Hubbard model.

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Entanglement spreading and quantum relaxation timescales with power-law decaying interactions

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We investigate the physical mechanisms underlying the spreading of entanglement in a quantum many-body system following an abrupt change of one of its control parameters -a quench. In particular, we focus on extended systems where the interaction among the microscopic building blocks decays as a power-law $1/r^{\alpha}$ at long distance. The buildup of correlations and entanglement in these systems has been studied a lot recently, mainly in connection with the breakdown of Lieb-Robinson bounds for sufficiently small alpha, and very paradoxical observations have been reported, for which no physical explanation has been put forward: while long-range interactions enable distant subsystems to become essentially instantaneously correlated, the growth of entanglement entropy in a subsystem is rather slowed down by long-range interactions. In this work, we propose a scenario resolving this paradox. We argue that the growth of entanglement entropy is a relaxation process involving time scales ranging from zero (for the fast modes) to infinity (for the slow modes), corresponding to the divergency of the velocity of the fastest quasiparticles for sufficiently long-range interactions. We support this scenario by analytical and numerical calculations on the long-range XY spin model.

An efficient way to determine a phase boundary

Kazuhiro Fuchizaki ¹, Yuta Asano ², Kazuma Okamoto ¹

An orthodox way to determine an equilibrium phase boundary is to look for the thermodynamic conditions under which the free energies of the two phases under consideration equilibrate. However, the evaluation of a free energy is usually not an easy task. two-phase simulation method [1] has been proposed to avoid such a time-consuming step of free-energy evaluation. Here, we propose a new type of the two-phase simulation method with which to estimate effectively the location of a solid-liquid phase boundary. The modified Lennard-Jones (mLJ) system was chosen because the accurate melting points are known as a function of pressure [2]. One of the methods is to apply the nonequilibrium relaxation (NER) method [3]. A combined system consisting of solid and liquid states was prepared as a proper initial state. On the solid side, 13500 particles with the reduced density 1.0 were located on the face-centered cubic lattice points whereas 14196 particles with the density 0.7 located on the face-centered orthorombic lattice points were taken to the liquid state using the isothermal-isobaric molecular dynamics simulation. The systems were then combined together to be evolved under isothermal and isobaric conditions. The density of the whole system was monitored during the evolution. Whether the thermodynamic condition under consideration is in the solid or liquid state could be judged by observing the density is to increase or decrease. The error of the melting point was less than 1% at the highest pressure condition examined [4]. To our knowledge, this is the first successful realization of applying the NER method to a system other than spin systems. A second method is to trace the phase boundary by slowly varying the pressure or temperature in such a way that the solid-liquid interface within the combined system remains unmoved. The latter method also gave almost the same melting points as those

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A self-consistent-field calculation for open systems such as graphene monoxide

Badie Ghayami ¹

To introduce a method for calculating the graphene monoxide(GMO) optical properties. Dielectric function of GMO is calculated using a self-consistent-field Markovian master equation formalism(SCF-MMFE). In here, to employ this method to calculate the dielectric function, complex conductivity, also to obtain plasmon dispersion and propagation length for substrate.

GMO is considered by SiO_2 and hBN substrates. Calculating is shown dielectric function and plasmon dispersion what describe GMO optical properties.

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Machine Learning of Quantum Forces: building accurate force fields via "covariant" kernels

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In recent years, the construction of data-driven force fields via Machine Learning methods proved to be a promising route in order to bridge the gap between accurate (but slow) quantum calculations and fast (but unreliable) classical potentials [1,2,3].

I will present a new scheme [4] that accurately predicts forces as vector quantities, rather than sets of scalar components, by Gaussian Process (GP) Regression. This is based on matrix-valued kernel functions, to which we impose that the predicted force rotates with the target configuration and is independent of any rotations applied to the configuration database entries. We show that such "covariant" GP kernels can be obtained by integration over the elements of the rotation group SO(n). Remarkably, in specific cases the integration can be carried out analytically and yields a conservative force field that can be recast into a pair interaction form. The accuracy of our kernels in predicting quantum-mechanical forces in real systems is investigated by tests on pure and defective crystalline systems.

I will further discuss how such learning algorithm can be used to build a measure of complexity of physical systems. Indeed, this can be defined as the number of canonically sampled configurations needed to achieve low generalization error with high probability.

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Symmetry Breaking in the Formation of Two Clusters with the Nonlinear Mean Field Kuramoto Model

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The Kuramoto model is universally applicable to many weakly interacting systems, such as Josephson junctions. However, in many cases couplings which include higher harmonics are needed, such as those relating to electro-chemical oscillators and phi-Josephson junctions. In this study, we consider a global mean field synchronization model, called the nonlinear mean field Kuramoto model, where a finite number of phase oscillators are coupled via a global mean field which is a nonlinear function of the Kuramoto mean field. As observed first by Komarov and Pikovsky [1], identical oscillators with initial phase drawn randomly from a uniform distribution form two asymmetrical clusters under such a model. The distribution obeys a scaling law of N^1/2, showing that such a symmetry breaking is related to initial fluctuations. We attempt to find the source in the asymmetry through analytical method as well as numerical method. Analytically, we conducted linear stability analysis, and reformulated the Watanabe-Strogatz dynamical equations in the complex plane. The singularity in the Moebius transformation is analytically located, which provides a candidate for the singularity of the dynamics that we seek. The numerical simulation confirms the location predicted by theory, but it also confirms that statistical tools can't be applied to study the location of the singularity based on only the initial condtions, because the singularity cannot be obtained without integration. During the investigation, further properties of Watanabe-Strogatz variables and of the nonlinear mean field Kuramoto model were discovered to indicate several future paths to take for uncover-

ing this process of symmetry breaking.

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Nonequilibrium quantum XX spin chain under multisite Lindblad baths

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We present the study of nonequilibrium steady state (NESS) for a one-dimensional quantum XX spin chain, which can be mapped into a fermionic tight-binding model through the Jordan-Wigner transformation. To this end, we have modeled the interaction between the particles at the ends of the system and the heat/particle reservoirs, maintained at different temperatures or chemical potentials, by including Lindblad dissipators in the quantum master equation. The system-reservoir interaction is then generalized to an arbitrary number of particles at each end of the chain that are in contact with the reservoirs. An exact equation for the covariance matrix of fermionic operators has been obtained. From this procedure, we have analyzed the behavior of heat flux and particle flux through the system when the number of particles that are in contact with the reservoirs tends to the thermodynamic limit. In addition to numerical results for the covariance matrix equation, we have obtained analytical results using perturbation theory, in the limit in which the interaction between the particles in the chain is small. We have also obtained the Onsager reciprocity relations between heat flux and particle flux in this regime, from which we calculated the transport coefficients associated with the system.

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Exploring contact between out of equilibrium systems in steady states - The question of non-equilibrium Intensive Thermodynamic Parameters

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Although equilibrium thermodynamics is well established and universal, an equivalent theoretical framework remains to be built for non-equilibrium systems, at least for simple ones which are in a steady state. Oono & Paniconi (1998) and some years after, Sasa and Tasaki (2006) have developed a "Steady State Thermodynamics" (SST) which is exploring the general thermodynamic structure that steady state systems should obey. On the other hand, an analytic approach based on simple statistical systems has led to the definition of Intensive Thermodynamic Parameters (ITP) with respect to conserved quantities (Bertin, Martens, Dauchot and Droz (2007)). They play an analogous role as temperature or chemical potential at equilibrium. More recently, Pradhan, Seifert et.al. (2011) and Dickman et.al. (2014, 2015) have revived these studies with numerical simulations of driven lattice gas models. They have tested in particular the consistency of Sasa and Tasaki's SST by exploring the zeroth law that must be satisfied by intensive parameters. They have found that a thermodynamic structure is at best approximately verified.

This work aims to pursue in more details the investigation of the contact between steady state systems and to make the link between statistical approaches on one side, and Sasa and Tasaki's thermodynamical approach on the other side. In this poster, we will present theoretical results based on exact calculations on mass transport models, emphasizing the important role of contact dynamics in de-

termining the steady state reached by two systems in contact. Different possible definitions of the chemical potentials will be discussed, together with their consistency. These results also have important implications for the validity of the Sasa-Tasaki formalism.

Phase Space Crystals from Periodically Driven One-dimensional Systems

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Phase space crystals is a novel and mathematically rather challenging subject in physics. Phase space crystals can be created by driving suitable classical or quantum mechanical systems in a specific periodic way. In this way it is possible to create systems with a variety of effective Hamiltonians which are otherwise difficult to realize (such as quasicrystals), and they can be varied by tuning the driving parameters. Phase space crystals also provide a new way to study topological phenomena in physics. They differ from lattices in real space since their coordinate systems, i.e., the phase space, has a non-commutative geometry, which naturally produces phases like those arising from magnetic fields. In this way topological insulators, which have attracted much attention recently, can be engineered. Still another option provided by phase space engineering is a controlled transition between one-dimensional and two-dimensional crystals in an effective magnetic field. The famous Hofstadter-butterfly structure in the energy spectrum thus can be realized in onedimensional systems. The primary physical system to create phase space crystals are ultracold atoms in optical lattices.

Additivity of the potential of mean force: Mayer's theory and computer simulation

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Mayer derived in 1942 a certain number of equations for a one-component fluid using the grand canonical ensemble (GCE) [1,2]. These equations serve as the starting point for Mayer's integral equation theory and are the one-component equivalent of the McMillan-Mayer (MM) solution theory [3].

Due to the theoretical and practical interest about the thermodynamics of solutions, it is necessary to study first the one-component system. In this work the corresponding equations which relate the pressure, internal energy and density of the system between two different activities z and z^* , are obtained in terms of the potential of mean force and the pair correlation function. In the derivation the additivity of the potential of mean force is assumed. Molecular dynamics simulations [4] are used to check the influence of this additivity assumption in the calculation of thermodynamic properties by means of the pressure equation.

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Phase transition in detecting causal relationships from obervational and interventional data

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Analysing data of, e.g., gene-expression experiments, and modelling it via network-based approaches is one of the main data analysis tasks in modern science. A first step is to use the observation of correlation to infer the structure of the underlying network, for example in the context of the inverse Ising model. Although this is already a algorithmically hard problem, it becomes even more challenging, when one is even interested in causal relationships between the network entities. When just using correlations obtained from observational data, such causal relationships can only be resolved partially.

One way out is to include interventions to the system, e.g., by knocking out genes when studying gene expression. This allows, in principle, to get a grip on the causal structure of a system. Here, we model the data using Gaussian Bayesian networks defined on directed acyclic graphs (DAGs). By applying an approach which allows for multiple interventions in each single experiment and which takes large-scale interaction effects into account by calculating joint maximum likelihoods (MLs) for rather large (sub) networks, causal relationships can be detected, in principle, with high accuracy. The algorithm which achieves this needs on top of the ML calculation to sample different causal orderings, which induce different DAGs. We present a new Monte Carlo approach to sample orderings, which is based on approximating the full ML by probabilities of orderings of triplets. We show that this approximation is rather good and efficient. This allows us to study the quality of the causality detection as a function of the fraction of interventional experiments. We observe

a (information) phase transition between phases where the causal structure cannot be detected and where it can be detected. The transition point occurs roughly where only one intervention per network node is necessary.

Diffusion-limited erosion and its non-local meta-conformal symmetries

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Diffusion-limited erosion (DLE) is a paradigmatic member of a specific universality class of fluctuating interfaces, distinct from the familiar Edwards-Wilkinson and Kardar-Parisi-Zhang universality classes. Other members in this class include the terrace-step-kind model of vicinal surfaces and also the integrable XXZ chain, conditioned to large values of the stationary current.

Although the dynamical exponent of DLE is z=1, none of the known variants of conformal invariance can act as its dynamical symmetry. In d=1 spatial dimensions, the infinite-dimensional dynamic symmetry algebra of DLE is constructed explicitly and will be shown to be isomorphic to the direct sum of three loop-Virasoro algebras. The infinitesimal generators are spatially non-local and use the Riesz-Feller fractional derivative. Co-variant two-time response functions are derived and reproduce the exact solution of diffusion-limited erosion. The relationship with the terrace-step-kind model of vicinal surfaces and the integrable XXZ chain are discussed.

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Testing conformal invariance in near-critical colloidal suspensions

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Both the critical Casimir interaction between two colloids immersed in a critical medium as well as the according interaction between two plates confining such a fluctuating medium are governed by the scaling functions known from conformal field theory. They are two special cases of a vast variety of possible geometries which are all connected via conformal mappings. However, near criticality conformal invariance no longer holds true and the geometry of the system has an effect on the form of the according scaling functions. Assuming that the geometric scaling variable from conformal field theory is nevertheless sufficient in the scaling regime of a near-critical system, we use the exact critical Casimir interaction scaling function of the Ising universality class in cylinder geometry with variable aspect ratio and open boundaries to expand the predictions to colloidal suspensions. Therefore we discuss which length scale is suitable for the temperature scaling variable and compare our results with Monte Carlo studies of two-dimensional systems of colloidal particles with according boundary conditions.

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Time-Dependent Variational Monte Carlo Calculation of Out-Of-Equilibrium Dynamics of Lieb-Liniger Bosons

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We extend the time-dependent Variational Monte Carlo method to continuous-space quantum hamiltonians together with a systematic multi-body expansion of the many-body wave-function. The resulting variational description is applied to the Lieb-Liniger model of interacting one-dimensional bosons. We first show that ground-state properties can be obtained with high precision with ground state energies several orders of magnitude more accurate than previous variational approaches based either on Variational Monte Carlo or continuous Matrix Product States. Then, we study the out-of-equilibrium dynamics induced by a quantum quench in the interaction strength. Our variational Monte Carlo results for the dynamics of the pair correlation at contact are in good agreement with existing exact Bethe ansatz results available for a small number of particles and non-interacting initial states, but also enables the study of large particle numbers and general quench protocols. Analysis of the quench dynamics of a correlated initial state reveals that, far from "super"-integrable points, the long-term dynamics of local density fluctuations approach closely thermal equilibrium.

Multi-loop calculation of critical exponents in the model A of critical dynamics

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In this talk we will discuss multi-loop calculations in the model A of critical dynamic, which describes isotropic ferromagnets. The main object of interest in this model is dynamical critical exponent z, which governs the phenomenon of critical slowing down - an unlimited increase of the relaxation time of the order parameter approaching the critical point.

We apply renormalization group method to find this exponent at the four-loop approximation. We have developed a new method to significantly reduce the amount of computations by appropriate grouping of the diagrams. This method significantly reduce the number of integrands and transform them to more simple form. We've adopted Sector Decomposition method for models of critical dynamics and used it for a numerical calculation of the diagrams.

The results for dynamical critical exponent compared with other theoretical results and with experimental data.

Sharp Transitions in the Evolutionary Dynamics of Group Formation

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We introduce a simple model, based on the Evolutionary Game Theory, for studying the dynamics of group formation. The latter constitutes a relevant phenomenon observed in different animal species, whose individuals tend to cluster together forming groups of different size. Results of previous investigations suggest that this phenomenon might have similar reasons across different species, such as improving the individual safety (e.g. from predators), and increasing the probability to get food resources. Remarkably, the group size might strongly vary from species to species, and sometimes even within the same species. For instance shoals of fishes, herds of lions, and human groups (e.g. families), represent some examples of animal groups of different size and, considering human groups, one can find small tribes or even smaller groups, composed of very few members (e.g. 2). In the proposed model, agents are represented as spin vectors, whose value of each entry can be s = +-1, and they try to form homogeneous groups of different size, on varying a parameter named individual payoff. The latter represents the gain one agent would receive acting individually. In particular, agents have to chose if to form a group, receiving a group payoff, or if to play individually. The phase diagram representing the equilibria of our population shows a sharp transition between the 'group phase' and the 'individual phase', in correspondence of a critical individual payoff. In addition, we found that forming homogeneous groups of small size was easier than forming big groups. To conclude, we deem that the proposed model and related results constitute a support to the hypothesis that the phenomenon of group formation has evolutionary roots.

An Evolutionary Perspective on the Costs and Benefits of Innovation

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Innovation plays an important role in a variety of systems, from the evolution of animal species to the emergence of technology in the human society. In general terms, innovation is something new, and able to improve the benefits for a system, allowing the latter to evolve. In few words, innovation is an essential element that guaranties both the progress and breakthroughs. However, innovation has a cost, or is risky, so often individuals (and whole societies) can be afraid of it. Freeman Dyson few years ago wrote a very interesting paper entitled 'Birds and Frogs', with a direct reference to the community of mathematicians. In his view, birds are those that fly with their mind up to see the connections between different fields of knowledge, thus they can be considered as innovators. At the same time, frogs are those able to deeply analyze mathematical problems, and their role is essential to put into practice innovations. We deem that this metaphor, i.e. birds and frogs, be really suitable also beyond mathematics. Notably, while innovators are able to propose new and great solutions, conservators have the ability to transform innovations into something that can be really used in our society. For instance, if an innovative scientist proposes a new model but none of her/his collegues go trough it investigating all the details, the innovator does not receive 'citations' (or recognitions) and, in her/his community, none takes profit from the new results.

In general, a careful mixing of innovators and conservators is mandatory for succeeding, i.e. to produce new usable ideas in science, technology, and so on. In addition, while innovators can also propose nothing new for a long time, usually conservators are more likely to produce improvements on consolidated ideas. Thus, at least in terms of productivity, innovators represent even a risk for a society.

Starting from these observations, we introduce a simple evolutionary game for studying the dynamics of a population composed of agents that can play as innovators or as conservators. Agents change their behavior according to the payoff, i.e. the gain, obtained by the group they belong to (equally divided among all components). In particular, the payoff depends on the mixing of innovators and conservators in each group, and on a numerical parameter called 'award factor', whose role is representing the policies of a society towards research and industrial production.

One of the main results of numerical simulations indicates the existence of a critical threshold of the 'award factor'. In particular, values lower than the critical threshold lead the agent population towards an ordered equilibrium (i.e. only conservators survive). To conclude, we introduce an approach based on the framework of evolutionary game theory for studying a topic of increasing interest in different communities and sectors of our society.

Mixed-order phase transition of the contact process near multiple junctions

Róbert Juhász ¹, Ferenc Iglói ¹

The contact process is a basic stochastic lattice model of epidemic spreading or population dynamics. It displays a nonequilibrium phase transition between a fluctuating active phase and an absorbing phase, which is continuous in any dimensions and falls into the universality class of directed percolation. Discontinuous transitions are rare in low dimensional fluctuating systems; for the particular case of onedimensional systems with short-range interactions they are conjectured to be impossible. We demonstrated by numerical simulations that a suitable topology of the underlying lattice is able to induce a discontinuous local transition even with a simple dynamics such as the contact process. We have studied, namely, the local critical behavior near a multiple junction composed of M semi-infinite chains. As opposed to the continuous transitions of the translationally invariant (M=2) and semi-infinite (M=1) system, the local order parameter is found to be discontinuous for M> 2. The temporal correlation length is found to diverge algebraically as the critical point is approached, so the transition is of mixed order. Interestingly, the corresponding exponents on the two sides of the transition are different. In the active phase, the estimate is compatible with the bulk value, while in the inactive phase it exceeds the bulk value and increases with M. We proposed a scaling theory, which is compatible with the numerical results. According to a strong-disorder renormalization group analysis, quenched spatial disorder makes the transition continuous for M> 2.

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Quantum Monte Carlo Simulation of Antiferromagnetic Binary Alloy System with Random Exchange Interactions

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Finite temperature properties of the 1D Antiferromagnetic Binary alloy of the type A(p)B(1-p) with random spin-spin interactions have been investigated by means of a Quantum Monte Carlo (QMC) simulation based on stochastic series expansion method. First, thermal variations of heat capacity and susceptibility have been calculated for a small system with exact diagonalization and QMC simulation. Next, influences of the finite-size on the thermodynamic variables have been discussed. QMC results show that values of the spin-spin interaction terms and concentration p of the magnetic atoms play a crucial role on the system characteristics. A hundred of random configurations have been used for each simulation data for all system sizes.

Unified treatment of threshold ionsation and Cooper pair formation in 2-electron atoms.

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Within the framework of hyperspherical coordinates we solve analytically the wave equation neat total break-up. That leads to the problem solving a wave equation on a closed manifold with unknown boundary condition. We follow the nuclear drop model, and attribute forces on the boundary to surface tension. The surface is here the equator of a hemisphere which correponds to collinear particle configurations. We solve analytically the wave equation on the equator taking the fictitious force from equator tension into account. We obtain two types of solution: An incoming wave mode in which the electrons attract each other with zero total momentum. This strongly corelated electron pair is reflected from a turning surface. In the following outgoing mode of motion the pair decays. Below threshold this decay supreses all high double Ryberg sattes; above threshold this mode is the quantum version of the classical Wannier trajectory. for threhold ionization. Symmetry properties of the pair are discussed.

Two-step melting in Two Dimensions with Long-ranged forces

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Recent progress in global-balance Monte Carlo algorithms has allowed to confirm the essentials of the Halperin-Nelson-Young theory (KTHNY) for the 2D Melting problem with short-range interactions [1]. A key challenge in these simulations are large correlation lengths which could be overcome by a new class of Monte Carlo algorithms [2].

In this talk, I will show that the new Monte Carlo paradigm can be extended to include long-range forces (including periodic images) rigorously, without any truncation effects. The resulting algorithm improves on the scaling of Ewald summation [3].

The new algorithm allows to check the scaling predictions of KTHNY theory in the long-range limit, and complete the phase diagram of inverted power-law potentials, relevant for charged colloids, plasma crystals, and other systems.

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Bjerrum defects as topological charges and the residual entropy of ices

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The concept of the residual entropy of ice, i.e., the configurational entropy of proton disorder at zero temperature, was introduced by L. Pauling in order to explain the observed discrepancy between the calorimetric and spectroscopic values of the absolute entropy of water. The missing entropy term was calculated using three assumptions:

- (i) all ice configurations satisfy the Bernal–Fowler ice rules (these rules state that each oxygen is covalently bonded to two hydrogens, each oxygen forms two hydrogen bonds to two other oxygens, and there exists exactly one hydrogen between a pair of neighboring oxygens);
- (ii) all configurations have the same energy; and,
- (iii) the positions of hydrogens in the oxygen-oxygen bonds are uncorrelated.

In this contribution the residual entropy of ices (Ih, Ic, III, V, VI) and clathrates (I, II, H) is calculated assuming (i) and (ii). The Metropolis Monte Carlo simulations in the range of temperatures from infinity to a size-dependent threshold are followed by the thermodynamic integration. In addition, the entropy of ice III exhibiting partial disorder is calculated as the function of occupation probabilities. Violation of assumption (ii) is discussed.

It sometimes happens that a route to results is more interesting than the results themselves. Thus, we studied the interaction of Bjerrum defects (topological charges) as the function of temperature at two levels of approximation: the ideal solution and the Debye–H'uckel

theory. The finite-size effects in the residual entropy are then estimated as

$$S(N) = S(\text{thermodynamic limit}) + a/N + b \ln N/N + c/N^1.5,$$

where N is the number of molecules, a,b,c are constants and in 3D it holds c=0. This result enabled us to accurately extrapolate to the thermodynamic limit.

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Engines with ideal efficiency and nonzero power for sublinear transport laws

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It is known that an engine with ideal efficiency has zero power because a reverisible cycle takes an infinite time. However, at least from a theoretical point of view, it is possible to conceive (irreversible) engines with nonzero power that reach ideal efficiency. This is achieved by replacing the usual linear tranport law by a sublinear one and taking the step-function limit for the particle current (chemical engine) or the heat current (heat engine) versus the applied force.

Hybrid kinetic-liquid model of high-pressure gas discharge

Vasily Kozhevnikov ¹, Andrey Kozyrev^{* ¹}, Natalia Semeniuk^{† ¹}

As is known the direct solution of Boltzmann kinetic equation is of great interest for theoretical investigation of various gas discharges. Such approach gives the most important information about the discharge and its evolution by providing electron and ion distribution functions at given time point. The complete numerical solution of Boltzmann equations for multi-component gas discharge plasma is quite challenging even for one-dimensional problems due to high computational costs. That is the reason why gas discharges are usually described in terms of simplified moments models with drift-diffusion approximation or particle-in-cell (PIC) approaches with Main disadvantage of these techniques is Monte-Carlo collisions. that the description of fast particles (e.g. runaway electrons) is considerably difficult, especially for high pressures and strong overvoltages. For example, PIC method operates with restricted ensemble of macroparticles, so the accurate description of small portion of particles (like electrons with high energies) is simply unfeasible. Here we present the novel hybrid theoretical approach for the simulation of discharges in dense gases. Within its framework, both plasma hydrodynamics and kinetics methodologies are used in order to describe the dynamics of different components of low-temperature discharge plasma simultaneously. As a demonstration of current model advantages, we apply it to consider one-dimensional coaxial relativistic gas diode. Namely, in terms of our model it was shown that electrons power spectrum contains a group of electrons with the so-called "anomalous" energies (above the maximal applied voltage value) that were not correctly predicted before, but do exists it various experiments.

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Marginal dimensions of the Potts model with invisible states

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We reconsider the (q+r)-state Potts model with q interacting and r non-interacting (invisible) states. The model was recently introduced to explain discrepancies between theoretical predictions and experimental observations of phase transitions in some systems where the Z_q -symmetry is spontaneously broken. The number of invisible states r introduced into the model plays the role of a parameter that regulates the order of the phase transition. For the particular case q=2it had already been shown that on the square lattice the change occurs at large r (for d=2) and that $3 < r_c < 4$ within the mean field analysis [1]. Within the mean field approach, we give a more precise estimate $r_c(q=2)=3.65(5)$. Moreover, we find the novel mechanism of changing the order of the phase transition in the region 1 = q < 2. It is characterized by two marginal dimensions, r_{c_1} and r_{c_2} [2]. These dimensions indicate how the discontinuity in characteristics of the first order phase transitions emerges. The above region of q is relevant for description of bond percolation (q = 1), some intermediate values of q also are known to have physical realisations.

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von Neumann entropy in classical statistical mechanics

Roman Kremar ¹, Andrej Gendiar ¹, Tomotoshi Nishino ²

Entanglement is a property of the quantum system. It expresses correlations between various parts of the quantum system. For the bipartite division von Neumann entropy can be used as a measure of the entanglement. Correlations are enhanced in the vicinity of the phase transition point and therefore von Neumann entropy can be used for detection of quantum phase transitions. It has logarithmic divergences around them [1]. Using Suzuki-Trotter transformation we can map the one-dimensional quantum model to the two-dimensional classical statistical model. Using this mapping we can define classical analogue of von Neumann entropy. Expecting the same singular behavior we can use this quantity for detecting the positions of the phase transition. This approach has several advantages. Firstly it can be used for the inspection of the new model with very little knowledge about it. Secondly it can be used to obtain the central charge of the critical model and enhance the knowledge of the criticality. Corner transfer matrix renormalization group (CTMRG) [2] method is a great framework in which to define classical von Neumann entropy. We will present results from our study of various models. Toy model based on the truncated tetrahedron [3]. Generalized Widom-Rowlinson model [4]. Eight-vertex model in a field [5] the 6-clock model [6].

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Eight-vertex model in a field

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The eight-vertex model is generalization of the ice-type or six-vertex model. It was exactly solved by Baxter [1] for the case without a fields. It was shawn that universality hypothesis does not hold for this model. Special type of the universality was defined so called weak universality. Eight-vertex model with fields is not integrable, but prediction was made [1,2], that weak universality will be destroyed by switching on the fields. For almost forty years was this conjecture not tested. We decided to test it [3]. The general eight-vertex model on a square lattice was studied numerically by using the Corner Transfer Matrix Renormalization Group (CTMRG) method. The method was tested on the symmetric (zero-field) version of the model, the obtained dependence of critical exponents on model's parameters is in agreement with Baxter's exact solution and weak universality is verified with a high accuracy. We confirmed numerically the conjecture in a subspace of vertex weights, except for two specific combinations of vertical and horizontal fields for which the system still exhibits weak universality. The eight-vertex model can be mapped from electrical to magnetic representation. The model is usually studied in the magnetic representation, we will present results for electric representation were even weak universality does not apply, model is fully non-universal.

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Phase transition in the fracture process of heterogeneous materials under unloading

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We investigate the fracture of heterogeneous materials which emerges under unloading from a constant sub-critical load. Based on a fiber bundle model we show that depending on the rate of unloading the system has two phases, i.e. at slow unloading the gradual accumulation of damage leads to global failure giving rise to a finite lifetime of the sample, while rapid unloading results in partial failure with an infinite lifetime. Analytical calculations revealed that the transition between the two phases occurs at a critical unloading rate analogous to continuous phase transitions where the surviving intact fraction of the sample plays the role of the order parameter.

We show by computer simulations that fibers break in sudden burts generating crackling noise which can be registered experimentally by the acoustic emission technique. At the onset of unloading the stress relaxation is accompanied by a decreasing rate of bursts characterized by a power law functional form analogous to Andrade creep. In the regime of finite lifetime the initial slow down is followed by an acceleration towards global failure. We demonstrate that the increasing rate of bursts obeys the Omori law of earthquakes which has been found to describe the aftershock sequence after major events.

Analysing the correlation of the lifetime of the sample and of the time where the minimum burst rate is reached we pointed out a relation which can be exploited for the forecasting of the imminent gobal failure of the system.

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Dynamical symmetry breaking and phase transitions in driven diffusive systems

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We study the probability distribution of a current flowing through a 1D diffusive system, connected to a pair of reservoirs at its two ends. Sufficient conditions for the occurrence of a host of possible phase transitions both in and out of equilibrium are derived. These transitions manifest themselves as singularities in large deviation functions, resulting in enhanced current fluctuations. Microscopic models which implement each of the scenarios are presented, with possible experimental realizations. Depending on the model, the singularity is associated either with a particle-hole symmetry breaking, which leads to a continuous transition, or in the absence of the symmetry with a first-order phase transition. An exact Landau theory which captures the different singular behaviors is derived.

Large deviations algorithms applied to the simulation of extreme drag fluctuations on obstacles in turbulent flows.

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Turbulent flows are known to generate important fluctuations of local velocity and pressure. This fluctuations can have an important mechanical on immersed structures. It is common practice in the engineer community to study the flow around immersed structures using synthetic turbulent flows that do not render the physics of these extreme fluctuations. Furthermore, because these fluctuations are rare, there is no hope in generating them through direct numerical simulations. However, it is possible to bias the statistics of these fluctuations using techniques inherited from statistical physics, recently applied to dynamical systems. The cornerstone of such methods is large deviations theory. The application of such methods to turbulent flows allows one to generate rare fluctuations with a reasonable numerical cost, without having to modify the dynamics of the flow, generated through DNS. This presentation will feature the results of the application of this approach to a simple flow, serving as a proof of concept and thus paving the way to applications to complex systems, closer to industrial concerns.

Direct calculation of the critical Casimir force by simulation of a binary fluid

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I will discuss how critical Casimir effects can be accessed through direct numerical simulation of a model binary fluid as it passes through the demixing transition in the high density phase. Simulations were performed in the semi grand canonical ensemble, in which the fluid composition fluctuates at fixed density. In slab geometry, a critical pressure anisotropy is observed in which the force per unit area parallel and perpendicular to the confinement direction are differ-The measured anisotropy collapses into a universal scaling form closely related to that for the critical Casimir force. The critical Casimir force itself can be defined as the critical excess contribution to the generalized pressure function, $P_{\perp} - n\mu$, conjugate variable to volume changes at fixed density n, with P_{\perp} the pressure perpendicular to confinement and mu the chemical potential. In the context of existing experimental and numerical studies of the critical Casimir force, such an approach could open the way to dynamical and nonequilibrium studies.

On the disorder-driven transition in d=3 semimetals

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After discovering graphene the materials with relativistic-like spectrum of electronic excitations have become a popular subject which currently drives several hot topics in physics. Among them there are three dimensional materials which have been recently identified as Weyl semimetals and which provide a new universality class of phase transitions. The Weyl semimetallic phase is topologically protected against small perturbations such as presence of disorder. For a weak disorder, the system remains in a semimetallic phase: the density of states vanishes linearly at the band crossing, where electronic transport is pseudoballistic. However, for a critical disorder strength a transition occurs towards a diffusive metallic phase, characterized by a finite density of states at the nodal point [1]. This transition has been studied numerically and using renormalization group in $d=2+\varepsilon$ [2] without consensus on the values of the critical exponents. We reconsider this problem in view of relevance of disorder correlations and rare events. We find that the renormalization flow generates new terms in $d=2+\varepsilon$ and propose an alternative route based on 4 epsilon expansion [3]. Our method allows one to calculate the critical exponents in a systematic way opening an interesting perspective on several issues related to the transition. Besides, we show that in three dimensions, three scenarios are possible depending on the disorder correlations [4]. While the same transition is recovered for short range correlations, for disorder decaying slower than $1/r^2$, the Weyl semimetal is unstable to any weak disorder and no transition persists. In between, a new phase transition occurs. This transition still separates a disordered metal from a semi-metal, but with a new critical behavior that we analyze to two-loop order.

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Between Order and Disorder in Yang-Mills System

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The Yang-Mills systems are governed by nonlinear equations and so it is not a surprise if they have a chaotic behavior. But on the other hand, there are many examples of stable solutions of nonlinear field equations. So the question of order and disorder in the equations of Yang-Mills systems is not a trivial one. In the contest of particle physics, Matinyan and al, were the first to show that classical Yang-Mills system is a K-one. It has been conjectured by Nikolaevsky and Shchur that if chaos is present in the dynamics of homogeneous field, then it is present in the full field theory. This was confirmed in the Y-M field. In this work we consider a little bit complication: we add quantum to the previous study. We found that the quantum version of a Yang-Mills gauge theory returns to the classical case if one neglects the interference terms and thus it is writing as a system of two non-linear differential equations. We study this quantum version by using the Painlevé test to demonstrate that the theory is non-integrable and also with the use of the graphical procedure to make evident the sensitivity of the theory to initial conditions. Then we modelize the interference parts with a white noise term and transform the system to a couple of stochastic differential equations and study them using the Khasminski procedure. We find that our stochastic differential system has a unique solution that does not explode in a finite time.

Signatures of topological phase transition in 3d topological insulators from dynamical axion response

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Axion electrodynamics, first proposed in the context of particle physics, manifests itself in condensed matter physics in the topological field theory description of3d topological insulators and gives rise to magnetoelectric effect, where applying magnetic (electric) field B(E) induces polarization (magnetization) p(m). We use linear response theory to study the associated topological current using the Fu-Kane-Mele model of 3d topological insulators in the presence of time-dependent uniform weak magnetic field. By computing the dynamical current susceptibility, we discover from its static limit an 'order parameter' of the topological phase transition between weak topological (or ordinary) insulator and strong topological insulator, found to be continuous. The dynamical current susceptibility shows a sign-changing singularity at a critical frequency with suppressed strength in the topological insulating state.

Our results can be verified in current noise experiment on 3d TI candidate materials for the detection of such topological phase transition.

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Glassy dynamics and localization on complex energy landscapes: a random matrix perspective beyond mean field.

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Many disordered systems such as spin glasses and supercooled liquids exhibit a glass transition where, below some characteristic temperature, the dynamics slows down drastically, with relaxation time scales either diverging or at least becoming too large to measure. The system then falls out of equilibrium, e.g. because it gets trapped in the local minima of its potential energy landscape. One of the simplest models for the resulting slow relaxation and aging is the trap model by Bouchaud and others: the system is simplified to a point in phase-space hopping between local energy minima. Two main ingredients specify the phase-space evolution: the transition rates between neighbouring minima and the phase-space connectivity, which defines a network of allowed transitions between minima. Previous studies have explored the analytically tractable mean-field case [JP Bouchaud et al, 1995], where the network is fully connected, and related approximations [P Moretti et al, 2011]. Our work deepens the understanding of the trap model by investigating the effects of more limited phase-space connectivity. We focus on the spectral properties of the master operator, which govern the dynamics of the system, and leave to future investigations the study of e.g. two-time correlation functions.

In our study, transition rates only depend on the departing trap depth as in the original Bouchaud model: every transition effectively involves activation to the top of the energy landscape and then falling

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into the new state. We consider the paradigmatic case of finite phase-space connectivity given by a random regular graph, where every state has the same number of accessible neighbours. The main quantities of interest are the average eigenvalue spectrum, or density of states (DOS), and the average degree of localisation of states. We use the inverse participation ratio as a measure for localisation as it allows us to distinguish between two situations: localised eigenstates with a finite number of non zero components, and de-localised eigenstates with an extensive number of non zero components. Similarly one can distinguish between the total DOS, and the extended DOS, which only includes the de-localised eigenstates of the system.

We develop a general approach for the case of sparse phase-space connectivity by means of the cavity method; quantities of interest are evaluated numerically via a population dynamics algorithm. Following the cavity construction we are able to develop a simple analytical "high-temperature" approximation for the eigenvalue spectrum, where effectively one cavity iteration is performed at finite temperature starting from the infinite temperature solution.

Numerical results for the eigenvalue spectrum show good agreement with the high temperature approximation: slow modes exhibit a mean field-like trend, while fast modes appear to be strongly influenced by the network structure. Two localization transitions are found, one each at the left and right edge of the spectrum. The total DOS and the extended DOS indicate the effective coexistence of localised and de-localised states around these localization transitions.

Thermally-activated creep and fluidization in flowing disordered materials

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When submitted to a constant mechanical load, many materials display power law creep followed by fluidization. A fundamental understanding of these processes is still far from being achieved. Here, we characterize creep and fluidization on the basis of a mesoscopic viscoplastic model that includes thermally activated yielding events and a broad distribution of energy barriers, which may be lowered under the effect of a local deformation. We relate the creep exponent observed before fluidization to the width of barrier distribution and to the specific form of stress redistribution following yielding events. We show that Andrade creep is accompanied by local strain hardening driven by stress redistribution and find that the fluidization time depends exponentially on the applied stress. The simulation results are interpreted in the light of a mean-field analysis, and should help in rationalizing the creep phenomenology in disordered materials.

S. Merabia and F. Detcheverry, "Thermally-activated creep and fluidization in flowing disordered materials", EPL, in press 2016

Expansion Coefficients Evaluation of the Free Energy at High Temperatures using Micro-canonical Numerical Simulations.

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In statistical systems, the free energy can be expressed by infinite power expansions of the inverse temperature. In the canonical ensemble, the evaluation of the expansion coefficients requieres knowledge of the energy fluctuations, this implies a hard numerical effort. Furthermore, this calculations must be held in the limit where the temperature tends to infinite. However, it is observed that the equation of state in the micro-canonical ensemble S(U) has a maximum in this limit and it is a smooth function whose derivate can be fitted with a quadratic polynomial around this maximum. Using a method proposed in reference [1] it is possible to evaluate with high accuracy the inverse temperature curves as a function of the internal energy for fluids with square well potential. From here we can obtain reliable values for the expansion coefficients of the free energy expansion.

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Granular gas experiments to investigate Non-Equilibrium Steady States

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We present experiments in granular gases that allow to address topical issues of non-equilibrium statistical physics in a simple way. At macro-scale, we investigate processes where fluctuations dominate, in the same manner as in mesoscopic systems. Our system is based on a Brownian rotator embedded in a steady-state granular gas. This rotator is passively excited by the random shocks of the beads, but can also be forced from outside. Analysis of the work exchange with this NESS are compatible with the Fluctuation Theorem as well as the Fluctuation-Dissipation Theorem. These relations accoordingly allow to define a parameter kT_{eff} playing the role of temperature in this dissipative macroscopic system, similar as temperature k_BT in an equilibrium system. A very specific and fruitful feature is that $kT_{eff} \sim 10^{-7}J$, which is very large compared to $k_BT \sim 10^{-20}J$. Indeed measurements are easier and more precise, but interesting questions arise about the comparison of these quantities. We can couple the Brownian probes in distinct such systems and characterize transport of energy between energy reservoirs at different temperatures. (It is interesting to note that transport, linked to inhomogeneity, is a specific features of driven dissipative systems.) We can also vary the density of one of the gas systems, the other being kept constant, such that the mean flux is kept constant. The parallel between 'mesoscopic' systems at equilibrium and these NESS 'macroscopic' systems is to be further explored and validated, tackling the following questions. When the density of the gas is decreased, the dimensionality of the bath is reduced accordingly (influence of fluctuations is enhanced). In which way is this affecting the motion of the Brownian probe, and transport properties?

Out of equilibrium dynamics across a discontinuous quantum phase transition

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We study the off equilibrium dynamics of systems when they are slowly driven across a discontinuous (first-order) quantum phase transition, thus extending previous results on classical and quantum systems at continuous transitions. We show that a scaling behaviour arises when the quench time-scale is appropriately rescaled with the system's size. The scaling behaviour is due to the interplay between dynamics and finite-size effects, and is entirely encoded in the static properties of the transition. We support our findings by numerical real-time evolution data on the ferromagnetic Ising chain with parallel and orthogonal fields.

Andreev-Bashkin effect in superfluid cold-gases mixtures

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We study a mixture of two superfluids with density-density and current-current (Andreev-Bashkin) interspecies interactions. Coupled superfluids undergo a dynamical instability for some values of the relative superfluid velocity. Within the fluiddynamic framework, we find that the Andreev-Bashkin interaction perturbs the onset of the dynamical instability and the frequencies of out of phase low energy modes. Due to the recent advancements in the realisation and control of Bose-Bose and Bose-Fermi cold gases, the corrections due to the Andreev-Bashkin effect have good chances to be measurable with present technology.

Maximum Entropy Analysis of Potential-Driven Flow and Transportation Networks

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The concept of a "flow network" – a set of nodes connected by flow paths – unites many different disciplines, including electrical, communications, pipe flow, fluid flow, ground and air transportation, chemical reaction, ecological, epidemiological and human systems. Traditionally, flow networks have been analysed by conservation (Kirchhoff's) laws and (in some systems) by network mappings (e.g. Tellegen's theorem), and more recently by dynamical simulation and optimisation methods. A less well explored approach, however, is the use of Jaynes' maximum entropy (MaxEnt) method, in which an entropy - defined over the total uncertainty in the network - is maximised subject to constraints, to infer the state of the network. There is a well-established literature on the use of MaxEnt methods for the analysis of network structures (graph ensembles) subject to various configurational constraints, but mostly without consideration of flows or potentials on the network.

We present a generalised MaxEnt framework to infer the state of a flow network, subject to "observable" constraints on expectations of various parameters, "physical" constraints such as conservation laws and frictional properties, and "graphical" constraints arising from uncertainty in the network structure itself. The method invokes an entropy defined over all uncertainties within the system, including all flow and potential variables and any other unknowns. The analysis also requires new numerical methods for the iterative solution of systems with nonlinear constraints. The method is demonstrated by application to several example systems, including: (i) a 1140-pipe urban water distribution network in Torrens, Australian Capital Terri-

tory, subject to nonlinear frictional constraints; (ii) a 327-node urban electrical power distribution system in Campbell, Australian Capital Territory, including distributed power sources; and (iii) several simple transportation networks subject to conservation laws and routing or cost minimisation constraints.

Phases and colloidal quasicrystals of lipid A-phosphate structures

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Specific spatial organization of lipopolysaccharides (LPS) in biological membranes forming rafts are involved in a series of processes e.g. transport, fusion, microbial & viral entries with subsequent attenuating immune-regulating response on the interleukin, antibody and cellular events in humans. Although the LPS are large molecules, most of the biological activity rests on the activity of a small portion of the LPS molecules known as lipid A. Therefore, it has been also an intense target to construct specific antagonistic molecules in order to compete with the lipid A-receptor site to eliminate the endotoxic events [1]. This contribution relates to nm-scaled ordered assemblies of lipid A-phosphates in aqueous dispersions, uniquely as quasicrystals and their phase transitions. However, within the different observed phases the various lipid A-phosphates are randomly positioned and the system is both orientationally and positionally isotropic, when examined as a function of volume fraction (ø), temperature (T), nature of cations, pH, and ionic strength (I) [2]. Lipid A-phosphate clusters reveal an intermediate degree of order in which the clusters are randomly distributed, as observed in fluids, glasses and forming discrete colloidal crystals. These lipids A clusters show shapes of spheres, squares, pentagons and hexagons, and are elements of close sphere packing processes except for the pentagon. Nevertheless, this system change upon confinement and behaves now orientationally anisotropic, and will appear differently in different spacial directions. This influence can be both direct and indirect, to control the size, shape, structure, properties of the crystals formed,

and of the nature of the lipid A-phosphate or assembly [3]. Nonspherical lipid A-phosphate and approximants self-assembled to form body-centered and face centered cubic liquid crystals. A transition of lipid A-diphosphates is observed between phase-separated-fattyacid chains and a mixed honeycomb phase. Lipid A-diphosphate, their corresponding monophosphates form complex structures and colloidal crystals from stoichiometric mixtures of lipid A-diphosphate and their approximants. The development of vaccines to booster the host defense against pathogenic invaders provides a new opportunity for more effective vaccines. This was accomplished with complexes comprised of antagonistic and non-toxic lipid A-phosphate analogs. They formed by spontaneous self-assembly under controlled conditions. For lipid A-monophosphate, rhombodo-decadecahedra (Fd3m) packing was suppressed because of instability in the mean curvature between the tetrahedral & the octahedral nodes. Tetrakaidodecahedra packing showed only tetrahedral nodes; the tetrahedral angle could only be retained between all edges if the hexagonal faces of the truncated octahedron were changed. Quasicrystals exhibited noncrystallographic packing of non-identical lipid A-phosphate spheres. The spatial packing of these spheres was in either a cuboctahedron or an icosahedron. It was noted that the observed (3.3.4.3.4) was a crystalline analogue of the icosahedral quasicrystal. The tiling pattern of triangles (N3) and squares (N4) possessed a p4gm plane group. Another coded lipid A-diphosphate approximant showed an 8/3 ratio, with 6-fold symmetry and plane group p6mm. Both dodecagonal phases revealed a N3/N4 ratio of approximately 2.34. Because of bond-orientational order the direction of domains was classified into three orientations for the (3.3.4.3.4) tiling, but only two for the 8/3 approximants. The linear phason strain was quite small (0.02) and much slower than the phonon strain. A phase transition between the FCC phase and the quasicrystalline phases was followed by SAXS, WAXS measurements and also analyzed by HRTEM. The SAXS experiments suggest that the transition from the FCC phase (Fm m) to the Q12 and Q18 phases proceeds through rearrangements of the micelles in the (111) layers of the FCC phase resulting from a rearrangement by a 30° rotation of the (111) layers. For a multidomain structure consisting of the same number of 30o-rotated and -unrotated layers this would give rise to diffraction patterns with 12fold rotational symmetry in the [111] direction. Because of the six-

fold symmetry the stacking of alternate $0\circ;30\circ;0\circ;...$ -rotated domains is equal to a stacking of $0\circ;30\circ;60\circ;$ -rotated domains similarly to the structure of a smectic twisted grain boundary phase if the angle α between the layer normal in adjacent slabs is a rational P/Q number. The structural differences reveal strong changes in endotoxicity, not in the CMC [4], but strong in antibacterial and cellular response indicators.

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Critical behavior in the presence of an order-parameter pinning field

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We apply a recently advocated simulation scheme that employs a local order-parameter pinning field to study quantum critical phenomena in the two-dimensional square-lattice bilayer quantum Heisenberg model. Using a world-line quantum Monte Carlo approach, we show that for this model, the pinning-field approach allows to locate the quantum critical point over a wide range of pinning-field strengths. However, the identification of the quantum critical scaling behavior is found to be hard since the pinning field introduces strong corrections to scaling. In order to further elucidate the scaling behavior in this situation, we also study an improved classical lattice model in the three-dimensional Ising universality class by means of Monte Carlo simulations on large lattice sizes, which allow us to employ refined finite-size scaling considerations. A renormalization group analysis exhibits the presence of an important crossover effect from the zero pinning-field to a critical adsorption fixed point. In line with field-theoretical results, we find that at the adsorption fixed point the short-distance expansion of the order-parameter profile exhibits a new universal critical exponent. This result also implies the presence of slowly-decaying scaling corrections, which we analyze in detail.

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Cluster variational method for stochastic dynamics

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One of us has recently proposed [1] a generalization of the cluster variational method which can be used to study the out of equilibrium dynamics and the steady states of kinetic Ising-like model. Here we show that this approach provides a general framework in which several previous results of a mean-field nature are reproduced as particular cases and can be systematically improved. We consider applications to Ising-like models on various graphs, epidemic models on networks and asymmetric exclusion processes.

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Site Belief Propagation equations for sparse spin systems

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This work addresses the problem of the marginalization of the joint probability of a spin system.

These systems can be viewed in the framework of graphical models, which provide a convenient way of representing conditional dependence relations among large numbers of random variables. Specifically, each node s in an undirected graph is associated with a random variable σ_s , while the set of edges E is used to describe the conditional dependency structure of the variables.

Belief propagation is an increasingly popular method of performing approximate inference on arbitrary graphical models: the goal of belief propagation (BP), also called the sum-product algorithm, is to compute the marginal distribution $p_s(\sigma_s)$ at each node s.

Graphical models and message-passing algorithms defined on graphs comprise a growing field of research. Great part of the appeal of belief propagation lies in its optimality for tree-structured graphical models (models which contain no loops). In fact, for tree-structured graphical models, belief propagation can be used to efficiently perform exact marginalization. Specifically, the iteration (1) converges in a finite number of iterations (at most the length of the longest path in the graph), after which the belief (2) equals the correct marginal $p_s(\sigma_s)$.

Nevertheless, it is also widely applied to graphical models with cycles by following the same local message passing rules at each node and ignoring the presence of cycles in the graph; this procedure is typi-

cally referred to as loopy BP. In these cases it may not converge, and if it does its solution is approximate; however in practice these approximations are often good, as we will see.

The purpose of this work is to prove the goodness of BP in arbitrary sparse graphs representing famous spin systems (in particular we will con- sider the Ising model with positive and negative couplings, and a spin glass system). We will compare the results with a modification to the BP algorithm that we will call "Site Belief Propagation". The latter is an implementa- tion of BP that does not involve message exchanging but only an updating of some "site-parameters".

Nonequibrium response of stalling systems

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The celebrated fluctuation-dissipation relations (FDR) regulate the response of systems to a perturbation out of equilibrium, relating it to the spontaneous fluctuations at equilibrium. We show that FDRs still hold in nonequilibrium steady states, when the currents being perturbed vanish (stall) amidst the flow of other non vanishing currents, hence in a situation of only "local" equilibrium. By contrast, Onsager's symmetry is violated. We present a general theory based on the mathematics of Markov jump processes. When the observational currents are *phenomenological*, in the sense that many transitions in the configuration space of the system contribute to the same current, the validity of nonequilibrium FDRs rely on a property, that we call *marginal thermodynamic consistency*, which is more restrictive than the thermodynamic consistency granted e.g. by local detailed balance.

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Mechanical response of a nanopore saturated with fluid: molecular simulation results

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We present molecular simulations of a simple Lennard-Jones fluid saturating a deformable nanopore. The simulations allow to obtain the deformation of the nanopore as a function of the liquid pressure, in a way similar to what is done experimentally to measure the effective elastic moduli of the walls of the porous solid. The results show unexpected discrepancy between the observed deformation and that deduced from the direct stress-strain curves of the solid matrix. This effect is correlated with the fluid structure at the interface with the solid, and could be relevant to experimental data analysis.

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Fluctuation-dissipation relation in spin ice

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Over the last decade spin ice materials, such as Dy 2 Ti 2 O 7 , have been at the centre of attention in the frustrated magnetism community. In particular, the development of the so-called Dumbbell model, which pictures the low energy excitations as magnetic charges interacting through a magnetic Coulomb force, has provided an elegant way to study these materials, thanks to a mapping from the easy-axis Ising spins on the pyrochlore lattice to charges on the dual diamond lattice [1]. In parallel, some of the most signicant progresses in non-equilibrium statistical mechanics in the last twenty years have come from the study of the uctuation dissipation ratio when the system of interest evolves out of equilibrium [2]. However, there is still no such study for spin ice. We fill this gap here. Using numerical simulations with local dynamics, we focus on the violation of the fluctuation-dissipation relation after a thermal quench for several physical observables such as the magnetization, the density of charges or the energy. This allows us to identify an aging regime in which we can extract effective temperatures and other characteristics of non-equilibrium thermodynamics.

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Equilibrium statistical mechanics and energy partition for the shallow water model

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Geophysical flows are highly turbulent, and yet embody large-scale coherent structures such as jets and long lived vortices. Understanding how these structures appear and predicting their shape are major theoretical challenges. Equilibrium statistical mechanics is a powerful approach that describes with only a few thermodynamical parameters the long time behavior of the largest scales of those geophysical flows within the inertial limit. This approach has also been proven useful to describe self-organization in weakly forced-dissipated configurations. Previous applications of the theory led to successful description of the Great Red Spot of Jupiter, or of ocean rings and jets [1]. Because of essential theoretical difficulties, all those previous applications were up to now limited to quasi-geostrophic models. Here we generalize the equilibrium statistical mechanics theory to the more comprehensive shallow water system, including inertia-gravity waves and the possibility of energy transfers towards small scales, with the concommittant emergence of a large scale vortical flow [2]. This is a key step towards an understanding of the energy balance of geophysical flows. Using large deviation theory, we compute the entropy of macrostates for the microcanonical measure of the shallow water system. The main prediction of this full statistical mechanics computation is the energy partition between the large scale vortical flow and small scale fluctuations related to inertia-gravity waves. We introduce for that purpose a semi-Lagrangian discrete model of the continuous shallow water system, and compute the corresponding statistical equilibria. We argue that microcanonical equilibrium states of the discrete model in the continuous limit are equilibrium states of the actual shallow water system. We show that the

presence of small scale fluctuations selects a subclass of equilibria among the states that were previously computed by phenomenological approaches that were neglecting such fluctuations. We provide explicite computations of the equilibria within the quasi-geostrophic limit (strong rotation limit), taking into account the presence of small scale fluctuations. This allows us to discuss the important role of bottom topography and rotation to sustain a large-scale flow structure. We finally address the possible role of small scale dissipation and shocks within this framework, and geophysical applications of those results.

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Phase diagram of the spin-1 bilinear-biquadratic Heisenberg model with and without quadratic Zeeman effect

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Using recently developed algorithms for U(1) and SU(2) symmetric MPS with periodic boundary conditions (PBC), we investigate the phase diagram of the spin-1 bilinear-biquadratic Heisenberg (BBH) model with particular emphasis on the dimerized phase with and without quadratic Zeeman interaction. Lowest-lying states are calculated for the whole range of the parameter θ for the BBH model of 10-100 sites without Zeeman effect. The results for the energies agree well with predictions of the Bethe ansatz and previous DMRG calculations (in particular, we obtain with high precision the Haldane gap for bilinear point $\theta = 0$ and four lowest-lying states for the biquadratic point $\theta = -\pi/2$). Furthermore, the results for the string correlator of a system of 100 sites and extrapolated results for the dimerization correlator also agree with earlier infinite-system calculations (the latter is calculated from two lowest-lying spin-0 states with different quasi-momenta, which form a degenerate doublet in the thermodynamic limit).

The question of the existence of the nematic phase close to SU(3) symmetric point $\theta = -3\pi/4$ in the BBH model without Zeeman effect [1] is specifically addressed. To this end two extrapolated gaps are calculated: one between two lowest spin-0 states and the other between lowest spin-0 state and lowest spin-2 state. We confirm the absence of the nematic phase at least up to $\theta = -0.72\pi$. Furthermore, the bounds of the dimerized phase of the BBH model with quadratic Zeeman effect are determined, and the discrepancy of the results of

different groups [2, 3] is judged. Our results indicate that the transition to the large-D phase occurs at least at D=0.3 at the biquadratic point.

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Noise Amplification In a Topological Quantum Memory

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We prove a no-go theorem for simulating the Kitaev chain with a chain of superconducting qubits: we show that the noise strength for the topological qubit formed by the chain diverges as the square-root of the number of physical qubits. We find that, to minimize the rate of scaling, the chain must be operated as close as possible to the topological phase boundary. This phenomenon is universal in that it is independent of the bath spectral density.

Bose-Hubbard model with cavity back-action

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We investigate a one dimensional Bose-Hubbard model in a cavity with a cavity back-action. The back action create a long-range effective interaction between the particles. We consider the hard core boson limit. The hard core bosons can mapped to spins. In the spin language the effective long range interaction has an anti-ferromagnetic nature. The phase diagram was investigated by exact diagonalization and mean-field methods. The mean field equations are derived from variational principles, and give a good description of the phase diagram. There are a Mott-insulator (ferromagnetic) phase, an anti-ferromagnetic phase, a critical phase of the system. There might be also a supersolid phase.

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Higgs mode and conductivity in the vicinity of a quantum critical point

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Relativistic quantum field theories with O(N) symmetries play an important role in describing the low-energy sector of several condensed matter systems in the vicinity of a quantum phase transition. Using non perturbative RG techniques, we study zero temperature dynamical properties of O(N) field theory in two space dimensions. We investigate the excitation spectrum of the model and show that there is a well-defined "Higgs" amplitude mode in the ordered phase near criticality for N=2 and 3. In addition, we compute the conductivity at low frequencies and determine its universal properties. Based on our results, we conjecture that one of the components of the conductivity in the ordered phase is a "superuniversal" number and depends neither on the distance to the critical point nor on N.

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Susceptible-infected-recovered model with recurrent infection.

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We analyze a stochastic lattice model describing the spreading of a disease among a community composed by susceptible (S), infected (I) and removed/recovered (R) individuals. A susceptible individual becomes infected catalytically with infection rate b. An infected individual becomes spontaneously either recovered with rate c or susceptible with rate a. This model is a modification of the SIR model by the introduction of recurrent infection. In addition to the two processes of the SIR model, S + I -> I+ I and I -> R, the model displays a third process I -> S. In epidemiology terms, this model for a much larger than c can be seem as a model which can be understood as a simplified version for the spreading of a disease in which the process S-> I and I-> S occurs many times before the occurrence of the process I -> R, in which case the individual acquires a permanent immunization. The recurrent infection is relevant to those diseases for which the full immunization is achieved after the infection has been acquired more than once. This model also can be interpreted as a model in which there is a immunization, but there is a possibility that the individual dies. By rescaling the time it is possible to reduce the number of parameter to two. We thus introduce the parameters p and q, understood as the effective immunization and recovery rates, defined by p = a/b and q = c/b. The phase diagram (p-q) was obtained by means of simple and pair mean field approaches as well as by numerical simulations of the model defined on a square lattice. We found that the critical properties place the model in the DyP universality class except when the rate c vanishes, in which case the model reduces to the contact model. In this case, the model belongs

to the DP universality class. We remark that our numerical results indicate that the critical line goes continuously into the critical point of the contact model. Assuming that is the case, it was found that the axis-p is tangent to the critical line. If we interpret the model studied here as a contact process with the addition of the process I -> R, then we may conclude that the parameter c is a relevant parameter. That is, for c nonzero, the model leaves the DP universality class. The DyP universal critical behavior of the model found here confirms the idea that some modifications of a model does not change the critical behavior. Our results were published in Physica A 467 (2017) 21–29. We would like to thank the financial support from FAPESP.

Winning the competition: enhancing counter-contagion in SIS-like Markov processes

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In this stduy we introduce a new SIS-like model of network diffusion where the probability rate functions can depend not only on the states of the nodes neighborhoods but on the whole network state. The model allows also competitive scenarios, where there are two states both diffusive. In this framework, we propose an efficient dynamic algorithm, Generalized Largest Reduction in Infectious Edges (gLRIE), that enhances the counter-contagion by allocating treatments. The algorithm is generalized to the case of network with hierarchical cluster structure. We perform simulations for a large set of parameters on random and real networks and compare the results with competitors from literature. The same idea was also applied in the different setting of deterministic SIS model in metapopulation and analysed in the framework of optimal control theory.

Non-equilibrium dynamics of Ising-like systems at the critical point: a cuda implementation

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By means of Monte Carlo simulations of the critical Ising and Majority voter models with Glauber dynamics on two dimensional honeycomb lattices we found that the dynamic critical exponents for the Majority voter model are in good agreement with the reported values of the Ising model. We explain how the critical dynamic can be implemented correctly in the Majority voter model using cuda.

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Multifractal analysis and simulation of spatial chaos, applications to geophysics

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There have been many attempts to analyse and simulate the fluctuations of chaotic systems whose spatial extension is of prime importance, such as turbulence, weather and climate. This was done at first with mono/uni-scaling approaches (e.g. structure functions, rescaled range or spectral analyses), however multifractal techniques are required to grasp the fundamental feature of intermittency, to track and simulate the scaling singularities of the underlying equations instead of relying on numerical, scale truncated simulations of these equations (e.g. Royer et al., 2008, Lovejoy and Schertzer, 2013 for climate).

Domains of Multifractal fields can arbitrarily large, but on the contrary their codomains have been be 1D. This prevents to deal with the key question of complex component interactions and their non trivial symmetries. The latter are unfortunately indispensable to answer to challenging questions such as the climatology of (exo-) planets based on first principles (Pierrehumbert, 2013) or to fully address the question of the relevance of quasi-geostrophic turbulence and to define an effective, fractal dimension of the atmospheric motions (Schertzer et al., 2012).

Fortunately, considering the Lie algebra of stochastic generators of cascade processes enabled to generalize multifractals to arbitrarily large codomains, e.g. large dimensional manifolds. In particular, we have recently investigated the neat example of stable Levy generators on Clifford algebra that have a number of seductive properties, e.g.

universal statistical and robust algebra properties, both defining the basic symmetries of the corresponding fields (Schertzer and Tchiguirinskaia, 2015).

These properties provide the basis for a convenient multifractal calculus that should help to overcome current obstacles to the use of multifractal analysis and simulation at their full extent, in particular in geophysics.

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Local energy minima of the three-dimensional Edwards-Anderson spin-glass model

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Spin glasses like the three-dimensional Edwards-Anderson model show a proverbial 'glassy' behavior with very slow equilibration as the result of their rough energy landscape. I.e., an energy-function that contains a multitude of local minima or metastable states separated by energy barriers. We use a newly developed dynamical greedy algorithm [1] in combination with flat-histogram methods in order to sample the distribution of these minima and compare with theoretical predictions [2].

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KPZ equation for disordered out-of-equilibrium quantum systems coupled to a thermal bath

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In the last few years experimental progress in the area of out-ofequilibrium exciton-polariton gases [1] gave rise to several questions concerning the physical behaviour of Bose-Einsten condensates under pump and dissipation. Such systems can be theoretically described by a generalised Gross-Pitaevskii Equation (gGPE) in which complex coecients and noise enrich the equilibrium picture. An analytical mapping between gGPE and the Kardar-Parisi-Zhang(KPZ) equation has been demonstrated at long wavelength if the uctuations of the amplitude of the condensate are negligible with respect to the ones of the phase field. Hence one expects that the long-distance properties of driven-dissipative condensates belong to the KPZ universality class and a numerical proof was given in (1+1)D [2]. However an experimental observation of such mapping is still missing. An important feature of experimental set-up is the presence of unavoidable disorder due to cavity imperfections and phonons. In this work we develop a Keldysh field-theoretical approach and derive the gGPE- KPZ mapping taking into account the role of disorder and interactions with an external phonon-reservoir at thermal equilibrium; we furthermore perform numerical simulations to test our predictions.

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TOY MODEL OF GEOMETRICAL COMPETITION IN NEEDLE CRYSTAL GROWTH

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We present a simple dynamical model which is supposed to catch the main properties of a set of needle crystals (like, e.g., diamond needles) growing from a flat substrate. We consider needles which start growing at time zero in random directions from a set of randomly positioned seeds. Any collision of such two growing needles implies a tip of one needle hitting the body of another one. Our assumption is that on such a collision the needle whose tip hits another one stops growing ('dies'), while another one continues to grow unperturbed. We discuss properties of this model both for an unlimited uniform initial distribution of seeds (i.e., when one has an unlimited line or plane where seeds are distributed with fixed density), and a seed distribution with limited support (i.e., all seeds are located within a given interval or half-line).

In the unlimited case we were able to find

- scaling behavior of the density of growing needles and of their angle distribution as a function of time in both (1+1)D and (2+1)D;
- the exact upper and lower bounds on the needle angle/density distribution as a function of time in (1+1)D;
- asymptotic solution of a Boltzmann equation in (1+1)D, which contradicts these bounds showing that Boltzmann approximation does not works, as typical for one-dimensional systems.

For the case with final support in (1+1)D

- given that there was a finite initial number of seeds, we calculate the full probability distribution of the number of needles surviving at infinite time;
- given that one half-line is filled with a fixed density of seeds, and another half-line is empty, we estimate the average number of needles infiltrating the originally empty half-plane up to a given time.

Entanglement properties of lattice bosons from a variational wave function

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Entanglement is a defining characteristic of many-body quantum systems, expressing the degree of non-locality required by the description of the state of the system, and quantifying the amount of classical information demanded to faithfully reproduce the reduced state of any subsystem. The ground states of many-body Hamiltonians with short-range interactions are generically characterized by area-law scaling of entanglement entropies of a subsystem, implying that the classical information required to store the reduced density matrix is exponential in the surface of the subsystem itself - this aspect impairs scalable simulations with methods based on the explicit reconstruction of reduced density matrix, such as DMRG, in dimensions higher than one. A viable alternative is based on variational ground states explicitly exhibiting an area-law scaling of entanglement. Here we explore the entanglement properties of entangled plaquette states (EPS) [F. Mezzacapo et al, New Journal of Physics, 11, 083026 (2009)] representing a systematically improvable variational Ansatz for lattice boson models, and lending itself to an efficient optimization based on variational Monte Carlo. We evaluate the explicit dependence of the entanglement entropy on the number of coefficients in the variational Ansatz, and contrast the entanglement properties of local vs. nonlocal plaquettes in the EPS structure. Applying the EPS approach to a lattice boson model (the spatially anisotropic pi-flux triangular lattice) which bridges 1d and 2d physics, we investigate how the entanglement scaling reveals the effective dimensionality of correlations.

Paths counting on simple graphs: from escape to localization

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There is a variety of statistical problems in physics of wave and heat distribution in nonhomogeneous media, for which solutions of corresponding hyperbolic or parabolic equations are localized in the vicinity of some spatial regions. The questions related to localization occur often in polymer physics, where such localization occur due to the inhomogeneity of specific point-wise covalent interactions of the polymer chain with the underlying background. However, there is a class of problems for which the origin of localization is purely entropic and is caused exclusively by geometrical reasons.

We consider in details this phenomenon for polymer systems on graphs of specific topology. We study the localization of trajectories on tree-like regular graphs with a special vertex at the origin which has a coordination number (root degree)different from those of other vertices. The singularity analysis of the respective partition function of all paths leads to the dependence of the critical root degree on the degree of other vertices. The same results can be received by studying the spectrum of the adjacency matrix of these graphs.

We also ask the question whether one can expect localization in path counting problem on decorated star graphs, which are topologically very similar to star tree-like graph with one principal difference: all vertices of the decorated graph have the same vertex degree, being multiply linked to the neighbors.

Nonequilibrium phase transition properties and frequency dispersions of hysteresis curves of a cubic core/shell nanoparticle system: A Monte Carlo Simulation study

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Monte Carlo simulation based on Metropolis algorithm has been used to study dynamic phase transition properties of a cubic core / shell nanoparticle system under a time dependent oscillating magnetic field source. The ferrimagnetic Heisenberg nanoparticle is described on a simple cubic lattice with spin-3/2 ferromagnetic core which is surrounded by a spin-1 antiferromagnetic shell layer. An antiferromagnetic spin-spin interaction between core and shell spins is used at the interface of the particle. Our simulation findings indicate that dynamic phase transition temperature of the system gradually decreases when value of the external field amplitude increases. Moreover, particular attention has been devoted the hysteresis treatments of the system. For the first time, frequency dispersion of hysteresis loop area curves have been categorized into three distinct types in Ref. (1) for kinetic Ising model for infinite systems. Results obtained in our study suggest that this type of a classification is also valid and possible for the present finite core/shell system, namely, frequency dispersions can be categorized into three groups for a fixed temperature, which are labeled as type-I, -II and -III, respectively. The curves in type- I correspond to the dynamically ordered phase and their corresponding hysteresis loops are asymmetric treatment around the origin for all the studied frequencies. In type-II, the hysteresis curves change their shapes from symmetric one to asymmetric one with increasing field frequency for the selected values of external field amplitudes. Finally, in type-III, the system exists in the dynami-

cally paramagnetic phase and the hysteresis curves present symmetric shape around the origin. Hence, corresponding dynamic loop area curves as a function of field frequency have a single peak for considered values of the applied field amplitude.

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Dysonian dynamics of the Ginibre ensemble

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We study the time evolution of Ginibre matrices whose elements undergo Brownian motion. The non-Hermitian character of the Ginibre ensemble binds the dynamics of eigenvalues to the evolution of eigenvectors in a non-trivial way, leading to a system of coupled nonlinear equations resembling those for turbulent systems. We formulate a mathematical framework allowing simultaneous description of the flow of eigenvalues and eigenvectors, and we unravel a hidden dynamics as a function of a new complex variable, which in the standard description is treated as a regulator only. We solve the evolution equations for large matrices and demonstrate that the nonanalytic behavior of the Green's functions is associated with a shock wave stemming from a Burgers-like equation describing correlations of eigenvectors. We conjecture that the hidden dynamics, that we observe for the Ginibre ensemble, is a general feature of non-Hermitian random matrix models and is relevant to related physical applications.

Massively parallel Monte Carlo simulations with population annealing

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While Moore's law of semiconductors has ensured for over forty years that the next generation of processors works significantly faster than the current one, for the last ten years or so serial code has not seen any speed-up from new hardware which, instead, achieves performance improvements only from packing more and more cores onto a single die. As a consequence, scientists working with computer simulations need to move away from intrinsically serial algorithms to find new approaches that can make good use of potentially millions of computational cores. Population annealing, that was initially suggested by Hukushima and Iba [1] and more recently was studied systematically by Machta [2], is a sequential Monte Carlo scheme that is potentially able to make use of such highly parallel computational resources. Additionally, it promises to allow for the accelerated simulation of systems with complex free-energy landscapes, much alike to the much more well known replica-exchange or parallel tempering approach [3-6]. The relative performance with respect to such more traditional techniques, the appropriate choice of population sizes temperature protocols and other parameters, the estimation of statistical and systematic errors and many other features, however, are essentially uncharted territory. Here, we use a systematic comparison of population annealing to Metropolis as well as parallel tempering simulations for the Ising model to gauge the potential of this new approach, and we suggest a range of heuristics for its application in more general circumstances.

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Using Random Boundary Conditions to simulate disordered quantum spin models in 2D-systems

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Disordered quantum antiferromagnets in two-dimensional compounds have been a focus of interest in the last years due to their exotic properties. However, with very few exceptions, the ground states of the corresponding Hamiltonians are notoriously difficult to simulate making their characterization and detection very elusive, both, theoretically and experimentally. Here we propose a method to signal quantum disordered antiferromagnets by doing exact diagonalization (ED) in small lattice clusters using random boundary conditions and averaging the observables of interest over the different disorder realizations. To this aim we study the Heisenberg spin-1/2 model in an anisotropic triangular lattice (SATL), where the competition between frustration and quantum fluctuations might lead to some spin liquid phases (SL) as predicted from different methods ranging from spin wave mean field theory to 2D-DMRG or PEPS. Our method reproduces accurately the ordered phases expected in the model, signals disordered phases by the presence of a large number of quasi degenerate ground states and presents a relatively weak dependence on finite size effects.

A simulational study of exchange anisotropy in magnetic nanoparticles in the presence of dynamic magnetic fields

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Exchange anisotropy (or exchange bias) originating from the magnetic interaction between a ferromagnetic (FM) and an antiferromagnetic (AFM) structure is a fundamental physical effect [1,2], and it is utilized in fabrication of several spintronic devices such as magnetoresistive devices, magnetic sensors, and reading heads in magnetic hard disks. The phenomenon which is essentially observed in magnetic nanoparticles and thin films, is manifested as a vertical or horizontal shift in the hysteresis loops plotted in a plane of magnetization versus magnetic field strength. The parameters such as temperature, magnetic interactions in substance, nanoparticle radius (as well as the film thickness), and structural defects are the fundamental physical factors that have a direct impact on this phenomenon.

Dependence of exchange anisotropy on the factors mentioned above (temperature, magnetic interactions in substance, etc.) inspired a great deal of theoretical studies in the literature [3,4,5,6,7]. However, it is quite a challenge to control the aforementioned phenomena in real magnetic systems, since the nature of magnetic interactions, defects, and similar factors cannot be controlled externally. On the contrary, amplitude and frequency of externally applied oscillating magnetic fields [8] can be easily adjusted. Hence, application of this kind of magnetic fields on the material promises a more practical and effective way of controlling the exchange anisotropy and SP phenomena. As far as we know, there is not any theoretical or experimental approach dealing with dynamical aspects of the problem.

In this presentation, using Monte Carlo simulations, we will discuss our recent results [9] on the dynamic phase transition properties of magnetic nanoparticles with ferromagnetic core coated by an antiferromagnetic shell structure. Effects of field amplitude and frequency on the thermal dependence of magnetizations, magnetization reversal mechanisms during hysteresis cycles, as well as on the exchange bias and coercive fields will be presented, and the feasibility of applying dynamic

magnetic fields on the particle will also be discussed for technological and biomedical purposes.

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Fluctuation properties and effective temperature of strongly interacting 1d bosons after a quench

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We make use of the exact mapping of hardcore bosons onto free fermions to investigate their fluctuations properties in momentum space, both in the equilibrium Gibbs ensemble (GE), as well as in the generalized Gibbs ensemble (GGE) describing the long-time evolution after a quantum quench. For the system at equilibrium we test the validity of a fluctuation-dissipation relation connecting the momentum distribution gradient with noise correlations in momentum space. This relation offers a fundamental tool for primary thermometry in weakly interacting, homogeneous systems, and it is found to be useful for the thermometry of hardcore bosons as well, over a broad temperature range. We then turn to the GGE description of the post-quench stationary state, showing that a similar thermometric scheme can provide a close estimate of the effective temperature of the system, which is generally defined by matching the internal energy of the system after the quench with the thermal one. Our results demonstrate the effectiveness of primary noise thermometry in the GGE without previous knowledge of the equation of state of the target Hamiltonian, and offer detailed insights into the fluctuation properties of non-equilibrium stationary states realized by strongly correlated quantum systems.

Berezinskii-Kosterlitz-Thouless transition of ultracold atoms in optical lattice

Tadeusz Kopec ¹, Tomasz Zaleski

We study the behavior of interacting ultracold bosons in two – dimensional optical lattice. We use the quantum rotor approach to the Bose-Hubbard model to derive the effective phase-only Hamiltonian and calculate the Berezinskii-Kosterlitz-Thouless phase transition temperature. It appears that quantum nature of the problem manifested in strong dependence of the particle effective mass on the particle density has negligible effect on the bound vortex-antivortex phase-field configurations of the ordered state. Instead, it is mostly determined by the kinetic energy of atoms and the chemical potential.

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Statistical property of earthquakes network: study active and passive points

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Recent results in complex systems have indicated that network theory, which is known as graph theory in mathematics, is a powerful method to handle unsolved complex problems. Earthquakes manifest spatio-temporal complex behavior that can be studied using complex networks. It is so essential for these studies to construct an appropriate network. Then we use the statistical mechanics to study the property of such a network.

We propose a new combination method of Abe - Suzuki method [1] and Telesca - Lovallo method [2] for constructing earthquakes network. We divide a geographical region into small square cells that these cells cover the entire region without any overlapping. If an earthquake with any value of magnitude occurs in a cell, we identify it as a vertex of a network. Then for connecting links between vertexes we use the visibility condition. Indeed in our method two events are connected to each other if visibility condition holds true between them.

For Iran, California and Italy-Greece earthquakes we divide the longitudinal and latitudinal ranges into cells (cell sizes changes from 4km-220km). We show that the constructed networks are scale free and theirs degree distribution obey the q-exponential function which is used in non-extensive statistical mechanics [3]. The diagram of q parameter in terms of the cell size has a peak at 31km for Iran and 44km for California and Italy. Due to dependence of network characteristics on each other for cell sizes less than peak size, only one of the cell sizes is enough to describe the earthquakes network. We found that such model network results in both the Gutenberg-Richter and Omori laws.

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Also we find the universal behavior of links and nodes number with time for same areas and same resolution of Iran, California and Italy-Greece earthquakes. This behavior is power law and similar to Omori law but there are differences between them.

Furthermore, analogy to Darooneh- Lotfi [4] by using the concept of PageRank, we find the passive and active points in the geographical region of Iran.

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Sticking transition in a minimal model for the collisions of active particles in quantum fluids

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Particles of low velocity, traveling without dissipation in a superfluid, can interact and emit sound when they collide. We propose a minimal model in which the equations of motion of the particles, including a short-range repulsive force, are self-consistently coupled with the Gross-Pitaevskii equation. We show that this model generates naturally an effective superfluid-mediated attractive interaction between the particles; and we study numerically the collisional dynamics of particles as a function of their incident kinetic energy and the length scale of the repulsive force. We find a transition from almost elastic to completely inelastic (sticking) collisions as the parameters are tuned. We find that aggregation and clustering result from this sticking transition in multiparticle systems.

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Explicit computation of Reynolds stresses through statistical mechanics approaches

Eric Woillez ¹, Freddy Bouchet* ¹

It is extremely uncommon to be able to predict analytically, from first principle, the velocity profile of turbulent flows and being able to compare it to observations. The self organization of barotropic turbulence into large scale stable structures evolving much slower than the typical time of eddies offers a unique opportunity for such an achievement through non-equilibrium statistical mechanics approaches. Jupiter's jets are a unique example, offering both this simple dynamical setup and a large amount of observations. We model the dynamics of Jupiter's jets by averaging the dynamics of eddies, in a barotropic beta-plane model, and explicitly predicting the balance between Reynolds' stresses and dissipation, thus predicting the average velocity profile explicitly [2].

In order to obtain this result, we adopt a non-equilibrium statistical mechanics approach. We consider a relevant limit for Jupiter troposphere, of a time scale separation between inertial dynamics on one hand, and stochastic forcing and dissipation on the other hand. A kinetic theory based on a quasilinear approach has been proven to be self consistent and exact in this inertial limit [1], however not giving fully explicit results. Starting from this kinetic theory and assuming further that the forcing acts on scale much smaller than the jet scale, we obtain a very simple explicit relation between the Reynolds stress, the energy injection rate, and the average velocity shear, valid far from jet edges (average velocity extrema) [2]. A specific asymptotic expansion close to jet edges unravel an asymmetry between eastward and westward, velocity extrema. We recover Jupiter's jet specificities:

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a cusp on eastward jets and a smooth parabola on westward jets.

While obtaining such analytic theory of barotropic jet, in accordance with Jupiter's observation is extremely encouraging, it may not be sufficient to describe all the processes at hand on Jupiter's troposphere. We discuss possible future generalization to more comprehensive model, including for instance baroclinic instabilities.

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8:00 - 9:00 Registration

Soft-matter and biophysics I

09:00 - 09:50 **A. Zippelius**

09:50 - 10:10 W.Janke

10:10 - 10:30 K. Polovnikov

10:30 - 11:00 *Coffee break*

Soft-matter and biophysics II

11:00 - 11:40 E. Zaccarelli

11:40 - 12:00 F. Hucht

12:00 - 12:40 **S. Ciliberto**

13:00 - 14:30 Lunch

Quantum many-body systems

14:30 - 15:20 **Z. Hadzibabic**

15:20 - 15:40 G. Carleo

15:40 - 16:00 F. Igloi

16:00 - 16:30 Coffee break

Machine learning

& Neural networks

16:30 - 17:10 **L. Zdeborova**

17:10 - 17:30 M. Krasnytska

17:30 - 17:50 C. Lucibello

17:50 - 18:10 E. Katzav

18:10 - 19:00 Cocktail

Quantum out-of-equilibrium systems

09:00 - 09:50 J.-S. Caux

09:50 - 10:10 L. Foini

10:10 - 10:30 V.Eisler

10:30 - 11:00 Coffee break

Disordered quantum systems

11:00 - 11:40 P. Prelovsek

11:40 - 12:00 P. Sierant

12:00 - 12:20 A. Cuccoli

12:20 - 12:40 R. Whitney

13:00 - 14:30 Lunch

Active matter

14:30 - 15:20 **I. Giardina**

15:20 - 15:40 G. Briand

15:40 - 16:10 Coffee break

Interdisciplinary topics

16:10 - 16:30 D. Banerjee

16:30 - 16:50 K. Golden

16:50 - 17:10 F. Bouchet

17:10 - 17:15 Z. Burda

17:15 - 18:30 Posters

18:30 - 21:00 Dinner

Classical out-of-equilibrium systems

09:00 - 09:50 P. Sollich

09:50 - 10:10 J. De Nardis

10:10 - 10:30 A. Chiocchetta

10:30 - 11:00 Coffee break

Disordered classical systems

11:00 - 11:40 **K.J. Wiese**

11:40 - 12:00 K.Martens

12:00 - 12:20 I. Balog

12:20 - 12:40 T. Kopeć

13:00 - 14:30 Lunch

Frustrated systems

& Topological matter

14:30 - 15:10 **V. Simonet**

15:10 - 15:30 S. Powell

15:30 - 15:50 M. Modugno

15:50 - 16:40 J. Chalker

16:40 - 17:30 Farewell coffee









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