MECO 41 - Book of Abstracts

The 41st Conference of the Middle European Cooperation in Statistical Physics



courtesy: Kurt Bauschardt

Vienna, Austria 14-17 February 2016

















Preface

The first scientific meeting that was held in the spirit of the MECO conference series (and thus could righteously be called MECO1) took place in Vienna between February 28th and March 1st, 1974 at the "Erste Physikalische Institut" of the University of Vienna; it was opened by the late Walter Thirring, then head of the "Institut für Theoretische Physik". The official title of this conference was "International Seminar on Structural Phase Transitions" and was organised by "The cooperation", i.e., a group of scientists working in statistical mechanics, coming predominantly from central European countries. The program of this 1974-conference is shown below (decorated by some handwritten, complementary comments). The idea of MECO1 was to bring together scientists from countries of both sides of the iron curtain and to foster cooperation between the respective groups.

In subsequent years and in alternating order, the conferences of this series were then organised on either side of the iron curtain; the acronym MECO, standing for "Conference of the Middle European Cooperation in Statistical Physics", was coined at the third meeting that took place in Bled (Slovenia) in 1976. The series of meetings was only interrupted in 1992/1993 as a consequence of the war in Yugoslavia.

More than 40 years after MECO1, this series of conferences returns to Vienna, where it takes place now for the third time.

A brief look at the program of the first meeting provides evidence of the tremendous change that has taken place in the topics addressed in the scientific fields that are covered by the MECO series. The hot topics were then structural phase transitions and a theoretical method of renormalisation groups applied to phase transitions in condensed matter systems. Today, the dominant topic of

MECO41 has become soft matter (from a statistical physics point of view). Nevertheless, even at this conference, the MECO series continues with its tradition of covering a very broad spectrum of topics in statistical physics, ranging from the dynamics of financial markets to the physics of biological systems.

At the MECO41 we are looking forward to over 100 poster presentations as well as 26 contributed and 9 invited talks, two of which are "European Physical Journal" lectures, sponsored by Springer.

The organisers gratefully acknowledge support from various organisations (see logos on the preceding page) and are thankful for the invitation of the Mayor of Wien, Dr. Michael Häupl, to the "10er Marie", a typical Viennese Heuriger, where the Conference Dinner will take place on Tuesday, February 16th, 2016. Finally, we thank all sponsors for their generous financial support.

Christoph Dellago, Reinhard Folk, Gerhard Kahl, Marcello Sega, and Stefan Thurner

Previous MECO conferences

1974 Wien (A) 1996 Bled (SL) 1975 Regensburg (FRG) 1997 Szklarska Poreba (PL) 1998 Trieste (I) 1976 Bled (Y) 1999 Lutherstadt-Wittenberg (D) 1977 Unterägeri (CH) 1978 Boszkowo (PL) 2000 Pont-a-Mousson (F) 1979 Trieste (I) 2001 Prague (CZ) 1980 Budapest (H) 2002 Sopron (H) 1981 Saarbrücken (FRG) 2003 Saarbrücken (D) 1982 Wien (A) 2004 Bratislava (SK) 1983 Bled (Y) 2005 Cortona (I) 2006 Primosten (CR) 1984 Gernrode (GDR) 1985 Aussois (F) 2007 Ladek Zdroj (PL) 1986 Liblice (CZ) 2008 Puchberg/Wels (A) 1987 Poidoux-Chexbres (CH) 2009 Leipzig(D)1988 Karpacz (PL) 2010 Pont-a-Mousson (F) 1989 Siena (I) 2011 Lviv (UA) 1990 Balatonfüred (H) 2012 Tatrianske Matliare (SK) 1991 Duisburg (D) 2013 Trieste (I) 2014 Coventry (UK) 1994 Smolenice (SK) 1995 Puchberg/Wels (A) 2015 Esztergom (H)

Program of MECO I

Provisional Inogram The International Seminar on "Structural Phase Transitions" will be held in the Großer Hörsaal (Main Auditorium) of the I.Physikalisches Institut (First Physical Institute) of the University of Vienna (Strudlhofgasse 4, 9th District, Vienna, Austria) on February 28th and March 1st, 1974. (The main auditorium is located on the second floor (I.Stock) of the building) These meetings are coordinated by the "Coordenation" building.) These meetings are coordinated by the "Cooperation", a group of scientists primarily from Middle Europe. Thursday, February 28th, 1974 9:00 a.m. Opening, "Keynote" Address W.Thirring (Wien) (45min) (1) "Critical Phenomena at Structural Phase Transitions as Measured by Paramagnetic Resonance" K.A K.A.Müller (Zürich) (45min) (2) "Neutron Scattering Studies of the Structural Phase Transition in SrTiO3 and KMnF3" S S.M.Shapiro (Brookhaven) (45min) (3) "Galvanomägnetic, Band Structure, and Relevant Critical Properties of SrTiO₃ between 4.2 and 300 K" P.Frankus (Wien) (20min) 3:00 p.m. (4) "Critical Dynamics and Microscopic Theory of the Central Peak at Structural Phase Transitions" F.Schwabl(Linz) (45 min (5) "Molecular Dynamics Investigation of Structural Phase Transitions" (slowing down of cluster dynamic, giving size to central peak phenomena) T.Schneider (Zürich) (30min) (5) "Dynamics of a Simple Model for a Structural Phase Transition" P.Szépfalusy(Budapest) (30min) Friday, March 1st, 1974 9:00 a.m. (1) "Underdamped Soft Modes in Order-Disorder Systems" R.Bline (Ljubljana) (45min) (2) "An Introduction to the Renormalization Group Approach to Critical Phenomena" G.Jona-Lasinio (Padova) (45min) (3) "Renormalization Group Studies of Critical Phenomena at Structural Phase Transitions" (effect of long-range forces on critical behaviop) R.A.Cowley(Edinburgh) behaviopy (45min)

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 3:00 p.m. (4) "Monte Carlo Experiments on Critical Phenomena and Metastable States" (45 min) (5) "Mößbauer Studies Near a Phase Transition" S.Großmann(Marburg) (20 min)
(6) FILM-Cluster Formation, Critical Slowing Down, and Central Peak Phenomena T.Schneider(Zürich)

(20 min)-

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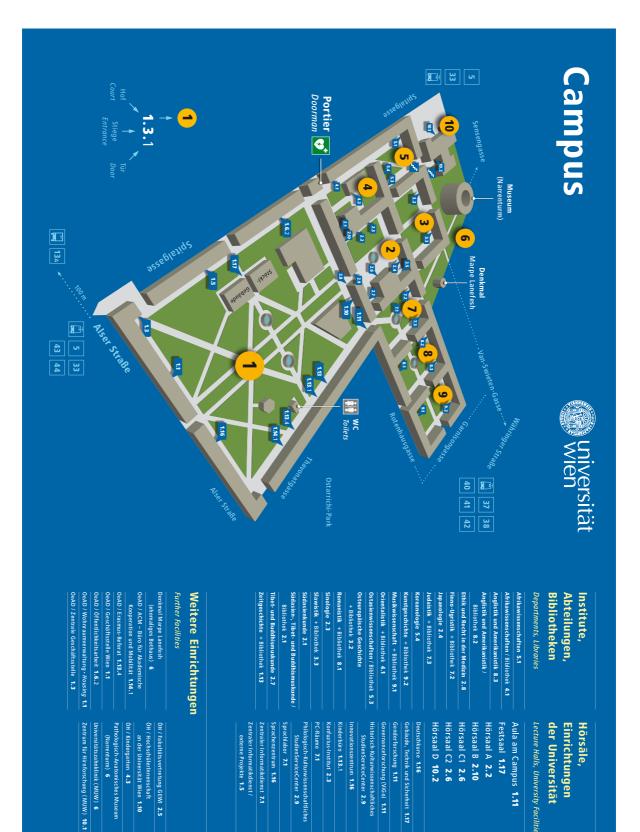


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Committees

Local Organising Committee

Christoph Dellago (University of Vienna) Gerhard Kahl (Vienna University of Technology) Marcello Sega (University of Vienna) Stefan Thurner (Medical University of Vienna)

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Welcome Reception, Dinner

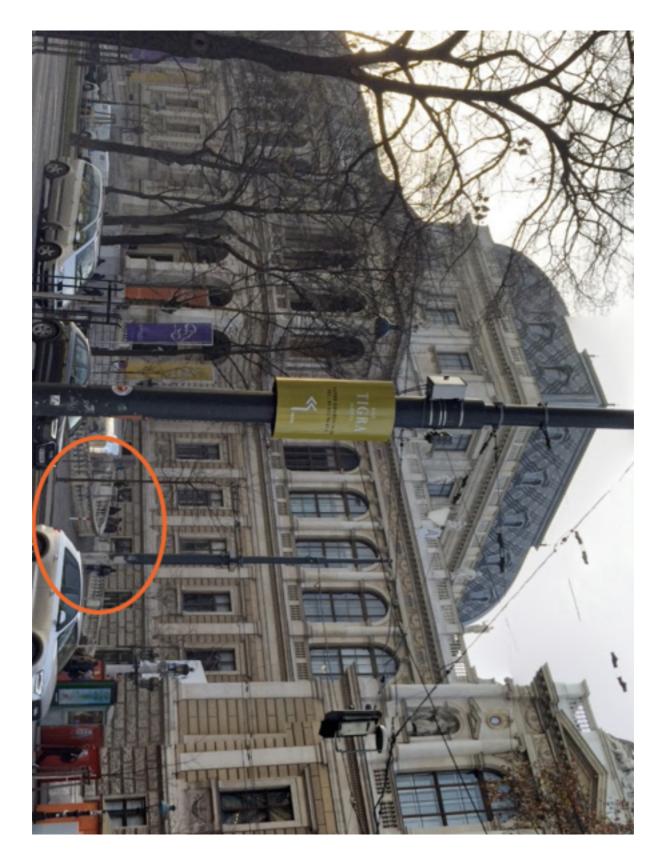
The Welcome Reception will take place on Sunday, February 13, 2016 from 18:00 to 20:00, in the foyer of lecture hall (Hörsaal) C in the Courtyard (Hof) 2 of the University Campus, Spitalgasse 2, 1090 Wien, Austria (see map on page 14). Snacks and drinks will be served.

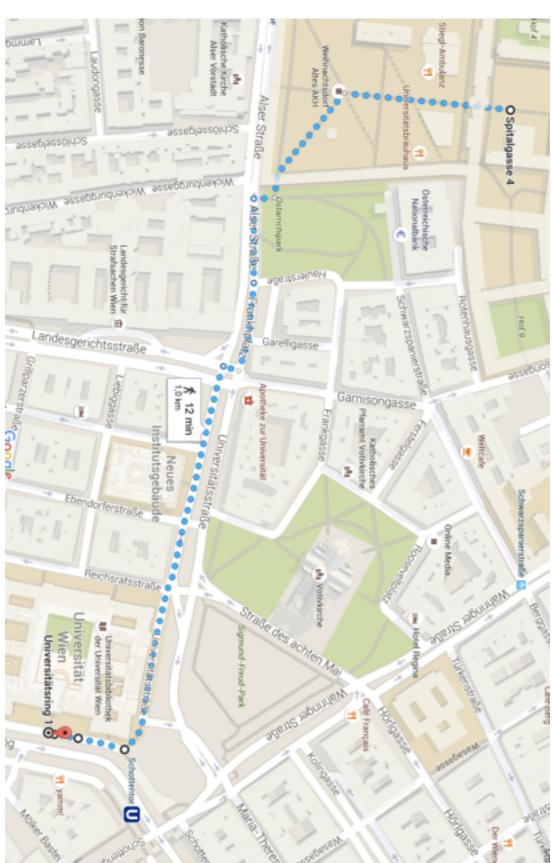
The Conference Dinner will be held on Tuesday, February 16th, 2016, at 19:00 at the Heuriger "10er Marie", located in Ottakringerstraße 222-224, 1060 Wien.

For Tuesday afternoon, we have organised an **Oldtimer-Tram touristic ride** that will bring the participants to the Heuriger, passing by some of the most famous sightseeings of Vienna around the Ring Road: Schwarzenbergplatz, Belvedere Castle, St. Charles's Church, Secession, the Technical University, the Town Hall, and many other.

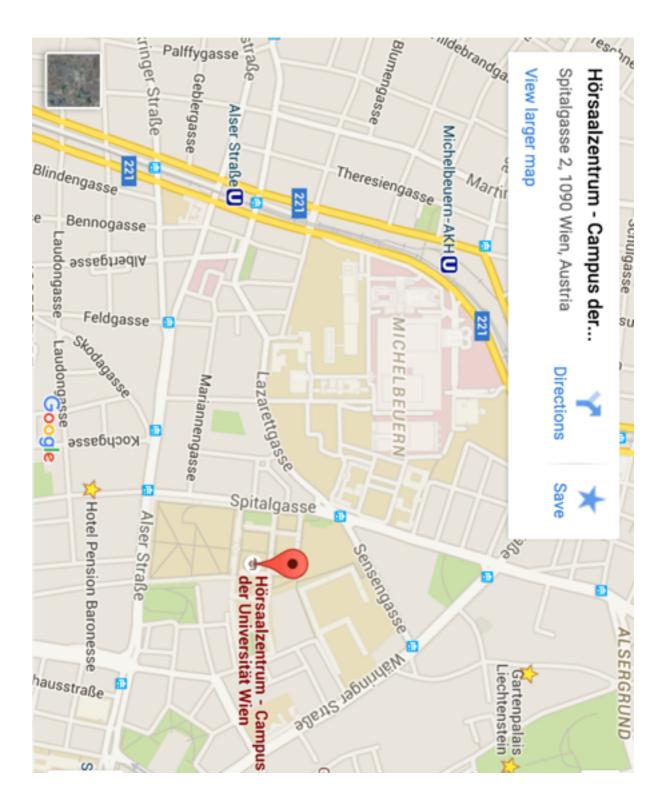
The meeting point for the tram ride is at 16:45 in front of the main building of the University of Vienna (Universitätsring 1, 1010 Wien). The train will bring us directly to the Conference Dinner.

Meeting Point for the Tram Ride Tuesday, February 16, 16:45





Meeting Point for the Tram Ride Tuesday, February 16, 16:45



Practical Information

Venue

The conference will take place in the lecture hall (Hörsaal) C in the Courtyard (Hof) 2 of the University Campus of the Universität Wien, Spitalgasse 2, 1090 Wien, Austria.

All lectures will be held in the lecture hall C1, close to the registration area. Poster sessions will take place in the foyer of the lecture hall.



Registration

The registration desk and the conference office are located at the entrance of the lecture hall (Hörsaal) C in the Courtyard (Hof) 2 of the University Campus of the University of Vienna. Registration starts on Sunday, February 14th, 2016 at 16:00; on this day the conference office is open from 16:00 to 20:00.

If you have not paid your conference fee yet, you will have the possibility to do so (in cash) at the conference office. On Monday, February 15th, 2016 the conference office opens at 8:00. On Tuesday and Wednesday our staff is available from 8:30 onwards at the conference office. The office closes on all days of the conference 15 minutes after the last lecture.

As you register you will receive the following documents:

- \clubsuit the conference booklet
- ✤ a name badge
- ✤ lunch coupons
- \clubsuit a letter certifying you attendance

All participants are kindly requested to wear their badge when attending the meeting; only participants who are wearing their name badges will be admitted to the lecture halls, coffee breaks and lunches. Further we emphasise that we can only admit registered participants wearing this badge to the conference dinner.

Oral presentations

Oral presentations will be given in the above mentioned lecture hall C. You can use your personal laptop for your presentation, however you are kindly asked to check half a day before your talk, if all details of your file are properly projected onto the screen. Please use preferentially coffee breaks for this check; our conference staff will provide you technical support. If you prefer to use our computer for the presentation, please notice that for technical reasons only ppt(x) and pdf files are accepted.

No overhead projectors will be available.

Plenary talks are scheduled for 40 (= 32 + 8) minutes, contributed talks are scheduled for 20 (= 16+4) minutes, including discussion as indicated in brackets. Chair persons are instructed to follow the time schedule rigorously.

Poster presentations

The poster sessions I and II will take place in the foyer of the lecture hall on Tuesday, February 16th and Wednesday, February 17th, 2016, from 14:00 to 15:20. Please check this conference booklet in the "Posters" section, to find out at which of the two sessions your poster will be presented, and which number has been assigned to your poster. The abstracts of the poster session are available online at http://meco41.univie.ac.at

The poster boards are 200 cm high and 100 cm wide. Adhesive tapes will be provided to fix the posters. Posters should be mounted in the morning and dismounted in the evening of the respective day. Posters that have not been dismounted in time will be removed by the organisers.

We kindly ask the presenters to stay close to their respective posters during the poster sessions.

Other useful informations

Internet

Dedicated Wifi connection will be available for all participants during the conference.

Wifi access through eduroam is also possible.

Coffee breaks, lunches

Coffee breaks will take place in the area close to the conference office and close to the exits of the lecture hall; please wear your name badge during coffee breaks, as only regular participants of the conference are entitled to participate in these breaks.

Lunches will be served for all participants at Stiegl-Ambulanz, located on Campus (Hof 1, see map below), at 2 minutes walk from the lecture hall. Lunch coupons will be provided at the registration.



Stiegl-Ambulanz (lunch)

Additional information

Conference staff will be happy to assist participants during the whole conference; members will carry special badges.

Possible changes in the program will be announced on a message board close to the conference office.

Program

Sunday, February 14

16:00-20:00	Registration		
18:00-20:00	Welcome Reception		

Monday, February 15

8:50-9:00	Opening
9:00-9:40	J. Yeomans, "Droplets bouncing on superhydrophobic surfaces"
9:40-10:00	M. Evans, "Model of antibiotic action on bacterial population growth"
10:00-10:20	T. Franosch, "Anomalous transport of circular swimmers in disordered structures: classical edge-state percolation"
10:20-10:40	Yu. Raikher, "Orientational Brownian motion in a viscoelastic ferrofluid. Magnetic and birefringence responses to ac field"
10:40-11:10	Coffee
11:10-11:50	H. Posch, "Hydrodynamics of one-dimensional particle systems"
11:50-12:10	T. Biro, "Master Equation for Random Network Dynamics"
12:10-12:30	P. Grassberger, "Percolation transitions in the survival of interdependent agents on multiplex networks, catastrophic cascades, and SOS"
12:30-12:50	H. Katzgraber, "Can we predict the difficulty of optimization problems without solving them?"
12:50-14:00	Lunch
14:00-15:20	Poster session I
15:20-16:00	E. Frey, "Evolutionary Games of Condensates" (EPJ Lecture)
16:00-16:20	F. Höfling, "Localisation dynamics of ballistic tracers in the two- dimensional Lorentz model interpreted as a renormalisation group flow"
16:20-16:50	Coffee
16:50-17:30	Yu. Holovatch, "Complex polymers: scaling and its
17:30-17:50	G. Delfino, "Interfaces near criticality"
17:50-18:10	J. Zierenberg, "Finite-size scaling of free-energy barrier in droplet formation and nucleation-like processes"
18:10-18:30	E. Ferrero, "Driving rate dependence of avalanche statistics and shapes at the yielding transition"

Tuesday, February 16

9:00-9:20	M. Schmiedeberg, "Mixing random organization and jamming"
9:20-9:40	H. Taitelbaum, "Mercury Droplet Spreading on Thin Metal Film on Glass: Statistical Physics of Advancing Interfaces"
9:40-10:00	V. Vlachy, "'Civilized' Model for Protein-Salt Mixtures in Water"
10:00-10:20	G. Steinbach, "Towards flexible and dynamic self-assembly from colloids with anisotropic interactions"
10:20-10:40	M. Oettel, "Marangoni flow and anomalous diffusion at interfaces"
10:40-11:10	Coffee
11:10-11:50	U. Seifert, "Stochastic thermodynamics and current fluctuations" (EPJ Lecture)
11:50-12:10	P. Maass, "Phase Transitions in Driven Diffusion and Brownian Motor Systems"
12:10-12:30	K. Kroy, "Fluctuation relations for a hot Brownian swimmer"
12:30-12:50	F. Pellegrini, "Markov State Modeling of Sliding Friction"
12:50-14:00	Lunch
14:20-14:40	A. Nikoubashman, "Directed assembly of soft colloids through rapid solvent exchange"
14:40-15:00	P. Jedlovszky, "Thermodynamic and dynamic properties at the intrinsic liquid surface"
16:45-18:45	Excursion
19:00	Conference Dinner

Wednesday, February 17

9:00-9:40	T. Loerting,	"Anomalous	Water:	One Substance,	Two	Liquids?"
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- 9:40-10:00 M. Ozawa, "Absence of the ideal glass transition in a binary Lennard-Jones glass former"
- 10:00-10:20 J. Horbach, "Computer simulation of glasses under shear: From inhomogeneous flow patterns to mechanical properties"
- 10:20-10:40 L. Filion, "Fabricating large two-dimensional single colloidal crystals by doping with active particles"
- 10:40-11:10 Coffee
- 11:10-11:50 C. Beck, "Nonequilibrium statistical mechanics approach to Lagrangian quantum turbulence"
- 11:50-12:10 W. Magnus, "A projection operator approach for the quantum canonical ensemble"

- 12:10-12:30 A. Ramsak, "Exact non-adiabatic qubit manipulation on Rashba rings"
- 12:30-12:50 R. Juhasz, "Random transverse-field Ising chain with long-range interactions"
- 12:50-14:00 Lunch
- 14:00-15:20 Poster session II
- 15:20-16:00 Z. Burda, "Reducing wealth inequality in macro-economic systems by introducing tax on wealth"
- 16:00-16:20 J. Smiljanic, "The associative nature of conference participation"
- 16:20-16:50 Coffee
- 16:50-17:30 P. Keim, "Spontaneous Symmetry breaking far from Equilibrium: Kibble-Zurek Mechanism in Colloidal Monolayers"
- 17:30 Closing

Invited Talks

Julia Yeomans (University of Oxford)



Droplets bouncing on superhydrophobic surfaces

Drops bounce easily on superhydrophobic surfaces because of low friction. We discuss how the design of the surface can affect the bouncing, leading to a droplet leaving the surface

shaped as a flattened disc or an extended cylinder. Lattice Boltzmann simulations and simple theories are used to help understand the reasons behind the unusual bouncing pathways.

Harald Posch (University of Vienna)



Hydrodynamics of one-dimensional particle systems

Linearized hydrodynamics of one-dimensional particle

systems is anomalous with respect to their dynamical properties. Taking the fluctuating Burgers equation as a starting point, we combine mode-coupling theory and exact results by Prähofer and Spohn [J. Stat. Phys., vol. 115, 255 (2004)] to derive asymptotic expressions for the time-correlation functions of the hydrodynamic modes and of their corresponding currents. The results are compared to extensive computer simulations for two simple fluids with short-range interactions. For the sound-mode sound-mode correlation function we find good agreement. The still persisting deviations for the current correlation functions are shown to be strongly reduced by going to larger systems and longer times. Erwin Frey (Ludwig Maximilians University of Munich)



Evolutionary Games of Condensates (EPJ Lecture)

Condensation phenomena occur in many systems, both in classical and quantum mechanical contexts. Typically, the entities that constitute a system collectively concentrate in one or multiple states during condensation. For example, particular strategies are selected in zero-sum games, which are generalizations of the children's game Rock-Paper-Scissors. These winning strategies can be identified with condensates. In our work, we apply the theory of evolutionary zero-sum games to explain condensation in bosonic systems when quantum coherence is negligible. Only recently has it been shown that a drivendissipative gas of bosons may condense not only into a single, but also into multiple non-degenerate states. This phenomenon may occur when a system of non-interacting bosons is weakly coupled to a reservoir and is driven by an external time-periodic force (Floquet system). On a mathematical level, this condensation is described by the same coupled birth-death processes that govern the dynamics of evolutionary zero-sum games. We illuminate the physical principles underlying the condensation and find that the vanishing of relative entropy production determines the condensates. Condensation proceeds exponentially fast, but the system of condensates never comes to rest: The occupation numbers of condensates oscillate, which we demonstrate for a Rock-Paper-Scissors game of condensates.

Yurij Holovatch (National Acad. Sci. of Ukraine)



Complex polymers: scaling and its manifestations

It is well known that the conformational properties of long

flexible polymer chains in a good solvent are governed by power laws (scaling laws). The search for these laws lead not only to the creation of modern theoretical physics and chemistry of polymers, but also enabled the discovery of a deep connection between the physics of critical phenomena and the physics of macromolecules. In this lecture, we discuss how do these laws change for polymers of complex topology (e.g. for polymer stars and networks), how they are modified under the influence of structural disorder (e.g. for polymers in crowded environment s in a cell or in a porous medium), how does the polymer composition influence the form of these laws. A theoretical description of the above phenomena is established via a field-theoretic approach involving renormalization group analysis. Our results find application in description of various physical, chemical, biological phenomena where these laws are manifest. These in particular include the description of phase diagrams of complex polymers, diffusion-limited catalysis and trapping reactions, multifractality of interacting random and selfavoiding walks, properties of proteins in crowded environment of biological cells, and the DNA helix-to-coil transition.

Udo Seifert (University of Stuttgart)



Stochastic thermodynamics and current fluctuations (EPJ Lecture)

Stochastic thermodynamics provides a framework for describing a large class of small driven systems. Examples are colloidal particles in time-dependent optical traps, single bio-molecules manipulated by optical tweezers or AFM tips, and transport through quantum dots. Thermodynamic quantities like work heat and entropy production can be identified on the level of an individual stochastic trajectory [1]. Non-equilibrium steady states are characterized by constant external driving through non-equilibrium chemical potentials or external forces or flows with a concomitant entropy production rate. I will discuss our recent work dealing with fluctuations in such NESSs. First, I will show how hidden slow degrees of freedom give rise to a "fine-structured" fluctuation theorem [2]. Second, I will show that constraining such fluctuations in order to have a more "precise" process inevitably requires a higher thermodynamic cost since for any isothermal process the product of its uncertainty and the free energy dissipated in it is larger than 2 kBT [3]. Finally, I will introduce a new class of constraints bounding extreme current fluctuations in arbitrary Markovian networks [4].

- [1] For a review: U.S., Rep. Prog. Phys. 75, 126001, 2012.
- [2] P. Pietzonka, E. Zimmermann, and U.S., EPL, 107, 20002, 2014.
- [3] A.C. Barato and U.S., Phys. Rev. Lett. 114, 158101, 2015.
- [4] P. Pietzonka, A.C. Barato and U.S., in preparation.

Thomas Loerting (University of Innsbruck)



Anomalous Water: One Substance, Two Liquids?

Water shows many anomalous properties, which includes its rich polymorphism and its "amorphous polymorphism". In this talk I will introduce the sixteen crystalline and three amorphous phases of ice. I will discuss how we prepare them in the laboratory, what their molecular structure is, where they can be found in nature, what kind of phase-transitions they can experience and how new ice phases were discovered in Innsbruck. I will discuss our experiments on the highly disputed question whether or not the amorphous phases are glasses in the sense of vitrified liquids. In fact, we recently achieved to observe coexistence of two glassy/ liquid water phases differing by 25% in density, which suggests that indeed a first order liquid-liquid phase



transition may be at the origin of the thermodynamic anomalies of water in the supercooled region. Furthermore, I will introduce some of our research, for which the properties of (deeply) supercooled liquid water play a crucial role, namely chemistry of water and aqueous solutions in the atmosphere and isolation of metastable intermediates by low-temperature solution chemistry. As an appetizer you can see the "popcorn ice effect" in the picture sequence, i.e., how high-density amorphous ice converts into low-density amorphous ice.



Nonequilibrium statistical mechanics approach to Lagrangian quantum turbulence

Many complex driven nonequilibrium systems are effectively described by a superposition of several statistics on different

time scales, in short a 'superstatistics'[1,2]. A simple example is a Brownian particle moving in a spatially inhomogeneous medium with temperature fluctuations on a large scale, but the concept is much more general. Superstatistical systems typically have marginal distributions that exhibit fat tails, for example power law tails or stretched exponentials. In most applications one finds three relevant universaliy classes: Lognormal superstatistics, chi-square superstatistics and inverse chi-square superstatistics. These can be effectively described by methods borrowed from nonequilibrium statistical mechanics. In this talk I will concentrate on some applications of this concept to better understand the statistics of tracer particles embedded in a) classical fully developed turbulent flows [3] and b) turbulent quantum liquids [4,5]. Some rigorous mathematical proofs generalizing these ideas to invariant densities of chaotic maps with slowly varying parameters have been recently obtained in [6].

[1] C. Beck and E.G.D. Cohen, Physica A 322, 267 (2003)

[2] C. Beck, E.G.D. Cohen, and H.L. Swinney, Phys. Rev. E 72, 056133 (2005)

- [3] C. Beck, Phys. Rev. Lett. 98, 064502 (2007)
- [4] C. Beck and S. Miah, Phys. Rev. E 87, 031002(R) (2013)
- [5] S. Miah and C. Beck, EPL 108, 40004 (2014)
- [6] C. Penrose and C. Beck, Dyn. Systems 31, 89 (2016)

Zdzislaw Burda (Jagiellonian University in Krakow)



Reducing wealth inequality in macro-economic systems by introducing tax on wealth

In his famous book 'Capital in the Twenty-First Century' Thomas Piketty argues that income tax is not able to reduce wealth inequalities because of the rate of return on capital is greater than the rate of growth of economy. He proposes to combine progressive income tax and wealth tax to prevent inequalities from further growing. In our talk we recall a simple model [by M. Mezard and J.-P. Bouchaud] of macro-economy represented as a network of trading agents. We extend the model by implementing taxation and redistribution to the system. We identify three basic regimes from the point of the influence of trade on wealth distribution:

- (a) self-stabilizing regime in which trade reduces inequalities
- (b) marginally stable regime in which trade weakly reduces inequalities
- (c) rich-gets-richer regime in which trade augments inequalities.

In each case we analyze the effect of income tax and/or wealth tax on wealth distribution. In particular we show that in case (c) any income tax and redistribution are not able to inhibit wealth inequalities from growing.

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Peter Keim (University of Konstanz)



Spontaneous Symmetry breaking far from Equilibrium: Kibble-Zurek Mechanism in Colloidal Monolayers

The Kibble-Zurek mechanism describes the evolution of defects and domains when a system is forced through a phase transition with spontaneously broken symmetry. It is used to describe transitions on such different scales like the Higgs field in the early universe shortly after the Big Bang [1] or in condensed matter systems like quenched quantum fluids [2]. Cooling at a finite rate, a domain structure naturally arises for a system with continuous phase transition. Since diverging correlation lengths are accompanied with critical slowing down, the system has to fall out of equilibrium for any non-zero rate in the vicinity of the transition. At this so called fall out time, a fingerprint of critical fluctuations is taken before the symmetry can switch globally. Within this picture, we investigate the non-equilibrium dynamics in a soft-matter analogue, a two-dimensional ensemble of colloidal particles which in equilibrium obeys the Kosterlitz-Thouless-Halperin-Nelson-Young melting scenario with continuous phase transitions. The ensemble is exposed to finite cooling rates of the pair-interaction parameter (being an inverse system temperature) at very different rates from deep in the isotropic fluid into the poly-crystalline phase. We analyze defect configurations as well as the evolution of orientationally ordered domains quantitatively via video microscopy and show that their frozenout length scale follows an algebraic decay as function of the quench rate as predicted [3].

- [1] T. Kibble, J. Phys. Math. Gen. 9 1387 (1976)
- [2] W. Zurek, Nature 317 505 (1985)
- [3] S. Deutschländer, Proc. Natl. Acad. Sci. 112 6925 (2015)

Contributed Talks

Model of antibiotic action on bacterial population growth Martin Evans (University of Edinburgh, Edinburgh, GBR)

Monday, February 15, 9:40-10:00

In this talk I will describe a simple model for the growth of a bacterial population under the challenge of ribosome-targetting antibiotics. The model is statistical physics-like in that it makes a coarse-grained description of the growth process, reduced to three variables within the bacterial cell - the antibiotic concentration, the concentration of ribosomes bound to antibiotics and the concentration of unbound ribosomes. Furthermore, there is biological input from empirically established physiological constraints which relate the three variables. Remarkably the model can explain several observations concerning antibiotic action and bacterial growth rate. In particular the growth-dependent bacterial susceptibility is controlled by a single, `universal' parameter and the extreme behaviours correspond to the phenomenological classification into bactericidal and bacteriostatic antibiotics. If time allows I will describe how the predictions of the model are backed up by experimental studies.

Anomalous transport of circular swimmers in disordered structures: classical edge-state percolation

Thomas Franosch (Innsbruck University, Innsbruck, AUT)

Monday, February 15, 10:00-10:20

Recently micron-sized self-propelled particles have been realized in the lab as model systems [1] for complex living organisms such as swimming bacteria. If the agent is asymmetric a natural circular motion [2] emerges which yields characteristic skipping orbits when interacting with confining boundaries.

Here, we investigate by event-driven molecular dynamics simulations the dynamics of circular swimmers in a two-dimensional model with randomly distributed scatterers [3]. For small radii of the swimming motion the agents orbit only around isolated clusters of scatterers, while at large radii diffusive behavior emerges.

For a certain critical radius a de-localization transition occurs which is generated by percolating skipping orbits along the edges of obstacle clusters. Directly at the transition the mean-square displacements displays subdiffusive transport.

The dynamic exponents associated with the transition differ significantly from those of the conventional transport problem on percolating systems, thus establishing a new dynamic universality class. This difference is tentatively attributed to a weak-link scenario, which emerges naturally due to barely overlapping edge trajectories.

We draw an analogy to the field-induced localization transition in magnetotransport in two-dimensional electron gases in a disordered array of antidots.

If time permits we also elucidate the conventional localization transition occcuring at high scatterer density and revisit universality as the microdynamics is changed from ballistic to Brownian dynamics [4]. There the splitting of the universality class is rationalized within renormalization group arguments for the probing of the narrow channels.

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[1] F. Kümmel, B. ten Hagen, R. Wittkowski, I. Buttinoni, R. Eichhorn, G. Volpe, H. Löwen, and C. Bechinger, Phys. Rev. Lett. 110, 198302 (2013)

[2] S. van Teeffelen and H. Löwen, Phys. Rev. E 78, 020101(R) (2008).

- [3] W. Schirmacher, B. Fuchs, F. Höfling, and T. Franosch, submitted
- [4] M. Spanner, F. Höfling, S.C. Kapfer, K.R. Mecke, G.E. Schröder-Turk,

and T. Franosch, accepted for publication on PRL

Orientational Brownian motion in a viscoelastic ferrofluid. Magnetic and birefringence responses to ac field

Yuriy Raikher (Ural Federal University, Ekaterinburg, RUS)

Monday, February 15, 10:20-10:40

A kinetic theory of rotary Brownian motion of dipolar particles suspended in a viscoelastic fluid is developed. The dipolar (magnetic) moment is assumed to be "frozen" in the particle body, and, for simplicity, the particle motion is taken to be one-dimensional (plane rotator model). The viscoelastic fluid is approximated by the Jeffreys model, which includes two friction mechanisms acting in parallel. One of them is Newtonian friction with the viscosity coefficient ηN , while another is Maxwellian friction with the viscosity ηM and retardation time $\tau M =$ nM /GM with GM being the elasticity modulus. The specifics of Maxwellian mechanism - it is modelled by a spring-damper sequence - is that at short times it mostly produces an elastic restoring torque (t $< \tau M$), while at long times (t > τM) its main effect is viscous friction. For an ensemble of such particles affected by thermal fluctuations (torques), the set of Langevin equations is obtained and then transformed to a rotary diffusion (Fokker-Planck) equation. Provided the interparticle interactions are negligible, this equation provides a well-defined description for the orientation kinetics of a viscoelastic ferrofluid. The kinetic equation is considered for the case of ac probing field and, to construct the solution, the orientational distribution function is expanded in powers of the field amplitude. In each order of such a perturbation theory, the statistical moments are expanded over a special set of orthogonal functions [1]. This approach enables one to consistently find, first, the linear response of the ensemble that renders the dynamic magnetic susceptibility, and then the quadratic response that renders the dynamic birefringence. Those functions are obtained in the form of chain fractions and, thus, are well fit for evaluation. The dynamic susceptibility, as expected, coincides with the one following from the linear response theory [2]. A compact analytical form for the dynamic birefringence (one may call it optical anisotropy susceptibility) of a viscoelastic ferrofluid is derived for the first time. Support of Project 15-12-10003 from Russian Science Foundation is gratefully acknowledged.

Master Equation for Random Network Dynamics **Tamás Biro** (MTA Wigner RCP, Budapest, HUN) Zoltán Néda (Babes-Bólyai University, Kolozsvár, Cluj-Napoca, ROU)

Monday, February 15, 11:50-12:10

We suggest a classification of random networks based on a simple, diffusion-like master equation. We view a network by its entries in the connectivity matrix, considering oriented and multiple connections in the general case. Generalizing further for real values in this matrix, flows on the network can be modeled. Based on a dynamics, changing the connection strength entries by one unit in a time-step, we classify the node-connectedness distributions via the stationary solutions of this master equation. From the simplest preference assumptions the Poisson, the binomial and the negative binomial (including the exponential) distributions emerge. Viewing subnetworks of huge network-environments thermodynamical principles can be easily recognized

Percolation transitions in the survival of interdependent agents on multiplex networks, catastrophic cascades, and SOS

Peter Grassberger (FZ Juelich, Juelich, GER)

Monday, February 15, 12:10-12:30

The "SOS" in the title does not refer to the international distress signal, but to "solid-on-solid" (SOS) surface growth. The catastrophic cascades are those observed by Buldyrev et al. in interdependent networks, which we re-interpret as multiplex networks with agents that can only survive if they mutually support each other, and whose survival struggle we map onto an SOS type growth model. This mapping not only reveals non-trivial structures in the phase space of the model, but also leads to a new and extremely efficient simulation algorithm. We use this algorithm to study interdependent agents on duplex Erdös-Rényi (ER) networks and on lattices with dimensions 2, 3, 4, and 5. We obtain new and surprising results in all these cases, and we correct statements in the literature for ER networks and for 2-d lattices. In particular, we find that d=4 is the upper critical dimension, that the percolation transition is continuous for d≤4 but — at least for d≠ 3 — in the universality class of ordinary percolation. For ER networks we verify that the cluster statistics is exactly described by mean field theory, but find evidence that the cascade process is not. For d=5 we find a first order transition as for ER networks, but we find also that small clusters have a nontrivial mass distribution that scales at the transition point. Finally, for d=2 with intermediate range dependency links we propose a scenario different from that proposed in W. Li et al., PRL 108, 228702 (2012).

Can we predict the difficulty of optimization problems without solving them?

Helmut G. Katzgraber (Texas A&M University, College Station, Texas, USA)

Monday, February 15, 12:30-12:50

Surprisingly often. Based on previous results of a large-scale numerical study of the equilibrium three-dimensional Edwards-Anderson Ising spin glass where it was demonstrated that autocorrelation times are directly correlated with the roughness of the free-energy landscape [Phys. Rev. E 87, 012104 (2013)], we show that a generalized spin-glass order parameter can be used as a proxy to the computational difficulty of various paradigmatic optimization problems. Our results are illustrated with different optimization algorithms and on a quantum annealer, as well as optimization problems. Furthermore, we show numerical evidence that the order-parameter distribution does mirror salient features in the free-energy landscape of complex systems for moderate system sizes. Finally, we corroborate and improve on these results using the family entropy of population annealing Monte Carlo [arXiv:1508.05647].

Work done in collaboration with Chao Fang, Richard Lawrence, Oliver Melchert, Humberto Munoz-Bauza, Andrew J. Ochoa, Wenlong Wang, and Zheng Zhu.

Localisation dynamics of ballistic tracers in the twodimensional Lorentz model interpreted as a renormalisation group flow

Felix Höfling (Freie Universität Berlin, Berlin, GER)

Monday, February 15, 16:00-16:20

The Lorentz model serves as a minimal model to explain many facets of the rich phenomenology of anomalous transport, as frequently observed in porous materials and cellular transport [1]. Here, I will discuss the localisation transition of "ballistic" tracers (subject to Newton's equations of motion) in the two-dimensional, overlapping Lorentz model. Extensive simulations provide evidence for the universality of the dynamic critical exponent, which has been crucial in the interpretation of recent studies [2,3]. The long-time asymptotes, however, are obscured by non-universal corrections to scaling, explaining the contradicting values for the diffusivity exponent in the literature. A spectral analysis of the obtained correlation flow of the transport at long times and gives insight into the fixed point structure of the RG flow.

[1] F. Höfling and T. Franosch, Rep. Prog. Phys. 76, 046602 (2013).

[2] S. K. Schnyder, M. Spanner, F. Höfling, T. Franosch, and J. Horbach, Soft Matter 11, 701 (2015).

[3] W. Schirmacher, B. Fuchs, F. Höfling, and T. Franosch, arXiv:1511.05218, Phys. Rev. Lett. in print (2015).

Interfaces near criticality Gesualdo Delfino (SISSA, Trieste, ITA)

Monday, February 15, 17:30-17:50

We present the exact theory of interfaces in near-critical planar systems at phase coexistence. The results include order parameter profiles, interface structure, passage probabilities and wetting properties, for the different universality classes and different geometries (strip, half-plane, wedge).

References:

[1] G. Delfino, J. Viti, Phase separation and interface structure in two dimensions from field theory, J. Stat. Mech. (2012) P10009.

[2] G. Delfino, A. Squarcini, Exact theory of intermediate phases in two dimensions, Annals of Physics 342 (2014) 171.

[3] G. Delfino, A. Squarcini, Phase separation in a wedge. Exact results, Phys. Rev. Lett. 113 (2014) 066101.

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Finite-size scaling of free-energy barrier in droplet formation and nucleation-like processes

Johannes Zierenberg (Institut für Theoretische Physik; Universität Leipzig, Leipzig, GER)

Philipp Schierz (Institut für Theoretische Physik; Universität Leipzig, Leipzig, GER)

Wolfhard Janke (Institut für Theoretische Physik; Universität Leipzig, Leipzig, GER)

Monday, February 15, 17:50-18:10

We study the nucleation free-energy barrier of the droplet formation process upon a temperature change. Employing generalized-ensemble methods allows us to directly access estimates of the free-energy barrier from energy probability distributions. Phenomenological arguments reveal that in this scenario the freeenergy barrier scales with $N^{1/2}$, confirmed by an extensive finite-size scaling analysis. The same scaling is supposed to remain true for other nucleation-like processes such as polymer aggregation. Driving rate dependence of avalanche statistics and shapes at the yielding transition

Ezequiel Ferrero (Universite Grenoble Alpes, Saint Martin d'Hères, FRA)

Monday, February 15, 18:10-18:30

In this talk I will first briefly introduce a coarse-grained approach for the study of amorphous solids under deformation, the so-called "elasto-plastic" models. Then, I will present some results from our study on avalanches statistics at the yielding transition.

We study the stress time series caused by plastic avalanches in athermally sheared disordered materials. Using extensive simulations of a mesoscopic elasto-plastic model, we find that critical exponents differ from mean-field predictions, that we approach only further away from the yielding point, at larger driving rates. We analyze the avalanche duration and size distributions introducing a scaling to account for the rate dependency of the dynamics. A probability distribution for local yielding is also discussed in the marginal stability picture and its driving rate dependence displayed. The average temporal shape of the stress drops also depends strongly on the imposed shear rate and system size. When individual avalanches are considered, they show a clear asymmetry.

Ref. arXiv:1506.08161

Mixing random organization and jamming

Michael Schmiedeberg (Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, GER) Moumita Maiti (Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, GER)

Tuesday, February 16, 09:00-09:20

By choosing appropriate protocols, both the random organization and the athermal jamming transition can be studied within a unifying model system [1]. We explore the model system for a mixture of the protocols and argue that the result is comparable to a glassy system of soft spheres at small but non-zero temperatures.

In our model system, we start with a random configuration of spheres. In order to obtain random organization, we displace overlapping particles randomly in each step. On the other side, athermal jamming is realized by deterministically shifting overlapping particles and heading for the local minimum of total overlaps without crossing energy barriers.

Finally, we mix these protocols. In case of mainly deterministic but also a few random displacements we obtain a system that corresponds to a system of soft spheres at small but non-zero temperatures. Therefore, we employ the model system to obtain insights into the differences between the glass transition at small but non-zero temperatures and the purely athermal jamming transition. For example, we determine the critical exponents of the transitions. Interestingly, the exponents of the random organization transition as well as the transitions in case of the mixed protocol correspond to the exponents from the universality class of directed percolation or conserved directed percolation, while athermal jamming seems to be a completely different transition.

Finally, we are interested in the relation to other transitions that occur in similar packing models, e.g., the contact percolation transition.

[1] L. Milz and M. Schmiedeberg, Connecting the random organization transition and jamming within a unifying model system, Phys. Rev. E. 88, 062308 (2013).

Mercury Droplet Spreading on Thin Metal Film on Glass: Statistical Physics of Advancing Interfaces

Haim Taitelbaum (Department of Physics, Bar-Ilan University, Ramat-Gan, ISR)

Tuesday, February 16, 09:20-09:40

When a droplet of mercury is transferred to a thin metal (silver / gold) film deposited on a glass substrate, it starts to dissolve and spread in a very non-trivial manner. This is the only known reactive-wetting system in room temperature. It exhibits two main regimes, the bulk propagation regime and the interface kinetic roughening regime. The bulk propagating dynamics is very different from classical wetting characteristics. In the kinetic roughening regime, rich spatio-temporal patterns are observed. The latter are studied and characterized using statistical physics tools, such as the growth, roughness and persistence exponents. We also discuss the decohesion and structural instability of the thin film due to the mercury penetration towards the metal-glass interface through the granular film structure. Various aspects of this complex sequence of phenomena will be addressed.

'Civilized' Model for Protein-Salt Mixtures in Water Vojko Vlachy (University of Ljubljana, Ljubljana, SLO)

Tuesday, February 16, 9:40-10:00

The effect of the nature of salt on properties of a model protein solution in water is studied theoretically and compared with experimental data. In our approach all the interacting species, proteins, ions of low-molecular-mass salt, and water molecules are accounted for explicitly (1). This is in contrast with the majority of other theoretical studies (see, for example, (2) and the Refs. therein), which treat the composed solvent as a structure-less continuum. The model proteins have simultaneously present positive and/or negative charges on the surface, mimicking this way the realistic situation occurring in such solutions. To solve numerically this complex model we utilize the associative mean spherical approximation, developed earlier for simple symmetric electrolytes and solutions of macroions (1,3). From measurable properties we choose to calculate the second virial coefficient, the quantity, which reflects stability of protein solutions and is closely related with the tendency of proteins to aggregate and crystallize. We show that osmotic second virial coefficient does not depend only on the magnitude of the net charge of the protein but also on its sign, as also on the nature of the present low-molecular-mass electrolyte. We find the specific ion effects to be correlated with differences in hydration free energy between the ions in solution and charged groups on the protein. The calculations capture experimental trends for lysozyme solutions reasonably well.

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2. M. Kastelic, Yu.V. Kalyuzhnyi, B. Hribar Lee, K. A. Dill, V. Vlachy, Protein aggregation in salt solutions, Proc. Natl. Acad. Sci. US.

3. Yu. V. Kalyuzhnyi, V. Vlachy, and K. A. Dill, Aqueous alkali halide solutions: can osmotic coefficients be explained on the basis of the ionic sizes alone? Phys. Chem. Chem. Phys., 12, 6260-6266 (2010).

Towards flexible and dynamic self-assembly from colloids with anisotropic interactions

Gabi Steinbach (Technische Universität Chemnitz, Chemnitz, GER) Dennis Nissen (University of Augsburg, Augsburg, GER) Manfred Albrecht (University of Augsburg, Augsburg, GER) Ekaterina V. Novak (Ural Federal University, Ekaterinburg, RUS) Pedro Sánchez (University of Vienna, Vienna, AUT) Sofia Kantorovich (University of Vienna, Vienna, AUT) Sibylle Gemming, (Helmholtz-Zentrum Dresden-Rossendorf, Dresden, GER) Artur Erbe (Helmholtz-Zentrum Dresden-Rossendorf, Dresden, GER)

Tuesday, February 16, 10:00-10:20

Colloidal particles are a suitable model system for the study of self-assembly and dynamic processes on the microscale. Here, we demonstrate the potential of anisotropic interactions between the particles for the design of complex networks with structural variability. The special feature of the presented approach lies in the presence of different types of connections in a homogeneous particle system. It enables the spontaneous formation of flexible architectures, which resemble the modular design of many biological systems.

As an example, we present a system of colloidal microspheres that have an offcentered net magnetic moment pointing perpendicular to the particle surface. They are an experimental realization of the theoretical model of spheres with radially shifted point dipole (sd-particles). Experimentally we observed the formation of branched structures as result of two coexisting self-assembly patterns, which is untypical for homogeneous systems. We show that the structural bistability can be explained by an extended model of sd-particles. This framework takes the broad and anisotropic magnetization distribution in the experimental particles into account.

We will further show that the interacting particles exhibit interesting nonequilibrium dynamics when exposed to time-dependent fields. Reversible structural reconfigurations emerge from the anisotropic interactions between the shifted net magnetic moments. The wealth of observable deformations and transformations particularly benefits from the complex self-assembly behavior. Marangoni flow and anomalous diffusion at interfaces

Martin Oettel (Universität Tübingen, Tübingen, GER) Johannes Bleibel (Universität Tübingen, Tübingen, GER) Alvaro Dominguez (Universidad de Sevilla, Sevilla, ESP)

Tuesday, February 16, 10:20-10:40

Collective diffusion for particles trapped at fluid interfaces is characterized by an anomalous speedup due to hydrodynamic interactions mediated through the bulk phases forming the interface [1]. Profiles at later times of an initial density fluctuation exhibit an intermediate range power-law decay in space which leads to diverging collective mean square displacements, experimentally signalled in a strong enhancement of the collective diffusion coefficient in the limit of zero wavenumber [2,3]. Confinement for particles and essentially unconfined hydrodynamic flow defines the notion of partial confinement.

In a wider interpretation, the diffusing particles at an interface are sources of a Marangoni flow which in turn acts back on its sources. Thus, the well-known spreading of soap films at interfaces is actually anomalous diffusion in the above sense. Furthermore, this anomaly always occurs when the lengthscale on which lateral spreading is observed is larger than the confinement width at the interface of the spreading particles or molecules. Therefore, anomalous diffusion is a rather general phenomenon, based on the presence of partial confinement.

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[2] B. Lin, B. Cui, X. Xu, R. Zangi, H. Diamant, and S. A. Rice,Divergence of the long-wavelength collective diffusion coefficient in quasi-oneand quasi-two-dimensional colloidal suspensions, Phys. Rev. E 89, 022303 (2014).

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Phase Transitions in Driven Diffusion and Brownian Motor Systems

Philipp Maass (University of Osnabrueck, Department of Physics, Osnabrueck, GER)

Tuesday, February 16, 11:50-12:10

In connection with directed transport on the molecular level, two research areas have attracted much attention in the past: Brownian motors and driven diffusion systems under a static bias. Brownian motors are operated by a periodic process in time, where, in contrast to classical engines, fluctuations caused by thermal noise and thermally assisted overcoming of energy barriers are important. Driven diffusion under a static bias has received particular interest in connection with transport through open tube-like compartments and for general studies of non-equilibrium steady states (NESS). I shall first address the problem of variables controlling NESS in the presence of particle interactions beyond hard-core repulsions and present a theoretical approach based on time-dependent density functional theory to predict boundary-induced bulk phases in generic situations [2,3]. Then I will show that boundary-induced phase transitions also appear in collective Brownian motors and argue that their occurrence is generic [3].

[1] M. Dierl, P. Maass, M. Einax: Classical Driven Transport in Open Systems with Particle Interactions and General Couplings to Reservoirs. Phys. Rev. Lett. 108, 060603 (2012).

[2] M. Dierl, M. Einax, P. Maass: One-dimensional Transport of Interacting Particles: Currents, Density Profiles, Phase Diagrams, and Symmetries. Phys. Rev. E 87, 062126 (2013).

[3] M. Dierl, W. Dieterich, M. Einax, P. Maass: Phase Transitions in Brownian Pumps. Phys. Rev. Lett. 112, 150601 (2014).

Fluctuation relations for a hot Brownian swimmer

Klaus Kroy (Institut für Theoretische Physik, Universität Leipzig, Leipzig, GER)

Gianmaria Falasco (Institut für Theoretische Physik, Universität Leipzig, Leipzig, GER)

Richard Pfaller (Institut für Theoretische Physik, Universität Leipzig, Leipzig, GER)

Tuesday, February 16, 12:10-12:30

Laser-heating of Janus particles provides a versatile nano-scale swimming mechanism with a great potential for technological applications. To characterize and control the dynamics of such hot nano-swimmers, one needs to understand both their enhanced Brownian fluctuations and their active self-thermophoresis. We performed non-equilibrium molecular dynamics simulations of a heated Janus bead in a Lennard--Jones fluid. They reveal some non-trivial spatiotemporal symmetries in the current statistics of the swimmer. In the Markovian limit, these can be cast in the form of analytically computable stationary fluctuation relations, in spite of the non-deterministic character of the driving and the strongly non-isothermal conditions.

Markov State Modeling of Sliding Friction

Franco Pellegrini (SISSA - Scuola Int. Sup. di Studi Avanzati, Trieste, ITA) Alessandro Laio (SISSA - Scuola Int. Sup. di Studi Avanzati, Trieste, ITA) Francois Landes (ICTP - Int. Centre for Theoretical Physics, Trieste, ITA) Santi Prestipino, (Universita' degli Studi di Messina, Messina, ITA) Erio Tosatti, (SISSA - Scuola Int. Sup. di Studi Avanzati, Trieste, ITA)

Tuesday, February 16, 12:30-12:50

Markov State Modeling has recently emerged as one of the key techniques for analyzing rare events in molecular simulations. In particular, in biochemistry this approach is successfully exploited to find the metastable states of complex systems in thermal equilibrium, such as a protein undergoing a folding event. We show that this technique can be exported to the study of friction, where strongly non-equilibrium events are induced by an external force. The approach is benchmarked on a Frenkel-Kontorova model, whose properties are well established. We demonstrate that the approach allows identifying the minimal basis of natural microscopic states necessary for describing the dynamics of sliding, including frictional dissipation and stick-slip events. We anticipate that the same technique can be applied to the analysis of realistic frictional systems. This work is supported by ERC Advanced Research Grant No. 320796 MODPHYSFRICT. Directed assembly of soft colloids through rapid solvent exchange

Arash Nikoubashman (Johannes Gutenberg University of Mainz, Mainz, GER)

Victoria Lee (Princeton University, Princeton, USA); Sosa, Chris (Princeton University, Princeton USA)

Robert Prud'homme (Princeton University, Princeton, USA)

Rodney Priestley (Princeton University, Princeton, USA)

Athanassios Panagiotopoulos (Princeton University, Princeton, USA)

Tuesday, February 16, 14:20-14:40

We studied the directed assembly of soft nanoparticles through rapid micromixing of polymers in solution with a non-solvent. Both experiments and computer simulations were performed to elucidate the underlying physics and to investigate the role of various process parameters. In particular, we discovered that no external stabilizing agents or charged end-groups are required to keep the colloids separated from each other, when water is used as the non-solvent. The size of the nanoparticles can be reliably tuned through the mixing rate and the ratio between polymer solution and non-solvent. Furthermore, we were able to fabricate a wide variety of patchy colloids, such as Janus particles, when polymer blends were used in the feed stream. Our results demonstrate that this mechanism is highly promising for the mass fabrication of uniformly-sized colloidal particles, using a wide variety of polymeric feed materials. Thermodynamic and dynamic properties at the intrinsic liquid surface

Pál Jedlovszky (ELTE University, Budapest, HUN) Balázs Fábián (Technical University of Budapest, Budapest, HUN) George Horvai (Technical University of Budapest, Budapest, HUN) Marcello Sega (University of Vienna, Vienna, AUT)

Tuesday, February 16, 14:40-15:00

Interfaces are ubiquitous objects, whose thermodynamic behavior we only recently started to understand at the microscopic detail. In computer simulations, when such interfaces are seen in atomistic resolution even the definition of the interface itself, in other words, the determination of the full and exact list of the molecules that are located right at the interface (i.e., at the boundary of the two coexisting phases) is not an obvious task at all. However, such a rigorous distinction between interfacial and non-interfacial molecules is a pre-requisite of any meaningful analysis of the interfacial properties. The development of various intrinsic surface analyzing methods in the last decade now enables us to discuss the thermodynamic properties associated with fluid ("soft") interfaces, such as the density, stress, energy, and free energy distribution across them by analyzing the respective contributions coming from successive layers. Also, having the successive subsurface molecular layers defined the variation of the dynamical properties of the particles along these layers can be discussed. In this presentation the basic concept of the identification of the molecules (ITIM) is explained, it is demonstrated how the distribution of the aforementioned thermodynamic quantities across the interface can be discussed both in terms of continuous profiles and in a layer-wise manner, several applications of this method is presented, and finally the diffusion of the interfacial molecules at the liquid water surface is discussed in detail.

Absence of the ideal glass transition in a binary Lennard-Jones glass former

Misaki Ozawa (Department of Physics, Nagoya University, Nagoya, JPN) Walter Kob (Universite Montpellier, Montpellier, FRA) Daniele Coslovich (Universite Montpellier, Montpellier, FRA)

Wednesday, February 17, 9:40-10:00

The dynamics of glass forming liquids shows a tremendous slowing down if temperature is decreased: Relaxation times, transport coefficients such as the diffusion constant or the shear viscosity grow by more than 15 orders of magnitude within narrow temperature range. One of the central goals in the field of glass physics is to understand the origin of this dramatic slowing down of the dynamics. There are several scenarios that seem to be able to explain the slowing down of the dynamics and the low temperature state of the glass former. A very popular one is to rationalize the slow dynamics by invoking the existence of a thermodynamic transition, the so-called ideal glass transition from the liquid to an ideal glass states. This ideal glass transition occurs when the configurational entropy, defined as the logarithm of the number of available states, becomes zero. Due to this singular behavior of the configurational entropy, the relaxation time and transport coefficients diverge if the transition point is approached [1]. However, confirming the existence of the ideal glass transition is a very difficult task since in practice the system falls out of equilibrium before reaching this putative ideal glass transition temperature, thus making the test of this theory most difficult. Furthermore, other scenarios are also able to explain the slow dynamics without resorting any thermodynamic transition [2]. In the present study, we investigate the existence of the ideal glass transition by using computer simulation of a canonical binary Lennard-Jones glass former in three dimensions. Massive computational effort and efficient sampling algorithm (parallel tempering) allow us to reach equilibrium states that are very deeply supercooled. By measuring the configurational entropy directly (obtained via thermodynamic integration), we find that the configuration entropy does not go to zero at a finite temperature. This implies that the thermodynamic singularity is indeed avoided before reaching a putative ideal glass transition temperature predicted by previous studies. Our results indicates that contrary to the previous results the system remains in a liquid state down to

zero temperature without showing an ideal glass transition. Furthermore, we analyze the microscopic structure and the potential energy landscape of the system to clarify the mechanism that leads to the avoidance of the ideal glass transition. We find that locally favored structures present in the liquid state hardly change in the temperature range we consider, which rules out another possibility for the slow dynamics, e.g. the transformation between two distinct liquids, so-called liquid-liquid transition [3]. Instead, we find the potential energy landscape contains extensive number of minima even very low temperature, which rationalize the avoided singularity. Our results support a theoretical argument that the ideal glass transition can not exist at bulk system in finite dimensions [5].

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Computer simulation of glasses under shear: From inhomogeneous flow patterns to mechanical properties

Jürgen Horbach (Heinrich-Heine-Universität Düsseldorf, Düsseldorf, GER) Gaurav Shrivastav (Heinrich-Heine-Universität Düsseldorf, Düsseldorf, GER) Pinaki Chaudhuri (The Institute of Mathematical Sciences, Chennai, IND)

Wednesday, February 17, 10:00-10:20

The response of glasses to mechanical loading often leads to the formation of inhomogeneous flow patterns that may strongly affect the material properties. Among them, shear bands, associated with strain localization in form of bandlike structures, are ubiquitous in a wide variety of materials, ranging from soft matter systems to metallic alloys. Molecular dynamics simulations of a model of a glass-forming binary Lennard-Jones mixture are performed to investigate the formation of shear bands, using different flow protocols. Under an externally applied constant stress, persistent creep in the form of shear-banded structures is observed around the yield stress, whereas under the application of a constant strain rate, shear bands occur at sufficiently low strain rates. For both cases, we give evidence that flow is initiated by a directed percolation transition. We analyze the nucleation of the shear-banded structures as well as the mechanical properties of the deformed glasses. Fabricating large two-dimensional single colloidal crystals by doping with active particles

Laura Filion (Utrecht University, Utrecht, NDL) Berend van der Meer (Utrecht University, Utrecht, NDL) Marjolein Dijkstra (Utrecht University, Utrecht, NDL)

Wednesday, February 17, 10:20-10:40

Self-propelled particles, also known as active particles, incessantly convert energy into self-propulsion, and as such are intrinsically out-of-equilibrium. While traditionally such particles occured solely within the purview of natural systems (e.g. bacteria), recent experimental breakthroughs have led to many novel types of synthetic colloidal swimmers. These systems exhibit a wealth of new phase behaviour, including motility-induced phase separation into dense and dilute phases, giant density fluctuations, and swarming. Moreover, experimental and simulation studies have shown that the dynamics of a passive system can be altered dramatically by incorporating as little as 1% of active particles into the system. At these concentrations, the self-propelled particles can be viewed as active ``dopants", which like passive dopants can strongly alter the properties (e.g. dynamics) of the underlying passive system.

In this talk I use simulations to explore the behaviour of two-dimensional colloidal (poly)crystals doped with active particles. We show that these active dopants can provide an elegant new route to removing grain boundaries in polycrystals. Specifically, we show that active dopants both generate and are attracted to defects, such as vacancies and interstitials, which leads to clustering of dopants at grain boundaries. The active particles both broaden and enhance the mobility of the grain boundaries, causing rapid coarsening of the crystal domains. The remaining defects recrystallize upon turning off the activity of the dopants, resulting in a large-scale single-domain crystal.

A projection operator approach for the quantum canonical ensemble

Wim Magnus (Universiteit Antwerpen, Antwerpen, BEL) Fons Brosens (Universiteit Antwerpen, Antwerpen, BEL)

Wednesday, February 17, 11:50-12:10

Constraining the particle number N in the canonical ensemble hampers the systematic calculation of the partition function Z_N for non-interacting fermions and bosons, unlike in the case of the grand-canonical ensemble, the reason being that the multiple summation over the single-particle states that involves products of Gibbs factors cannot be rewritten as a multiple product of sums over single-particle modes.

Recently, however, we have bypassed this difficulty and shown that the summation can be performed anyway by invoking a projection operator approach that automatically imposes the particle number constraint in the many-particle Hilbert space. Until now, only a recursion relation expressing Z_N in all partition functions of lower particle numbers is known to be available. The projection operator approach, however, provides a direct integral representation for Z_N as well as for the two-point and four-point correlation functions, thus reducing the old summation problem to a numerical integration task. As an illustration, the Helmholtz free energy and the chemical potential are computed for a twodimensional electron gas typically residing in the inversion layer of a field-effect transistor and the results are compared with those conventionally obtained from the grand-canonical ensemble. One of the conclusions is that the chemical potential not only emerges as a by-product of the calculation of the canonical partition function but may also take incorrect, unphysical values for low particle numbers when calculated within the grand-canonical picture. This new insight may be considered useful as such, but has also relevant consequences for the evaluation of the so-called sub-threshold slope of nano-scale transistors with few electrons, which is a hot topic today and which heavily relies on reliable values of the chemical potential and the gate metal work functions.

Exact non-adiabatic qubit manipulation on Rashba rings

Anton Ramsak (Faculty of mathematics and physics, University of Ljubljana, Ljubljana, SLO)

Wednesday, February 17, 12:10-12:30

First we will present exact solutions for an electron in a quantum wire with time dependent spin-orbit interaction and driven by external time-dependent potential [1,2]. By the virtue of the exact solution one can construct analytically the corresponding geometric Anandan phase or in the adiabatic limit the Wilczek-Zee phase, which enables holonomic qubit transformations. By breaking the time reversal symmetry the results lead to the Aharonov-Anandan phase and in the adiabatic limit reproduce the usual Berry phase. Next the result will be generalized and an exact solution will be presented for the timedependent wavefunction of a Kramers doublet which propagates around a quantum ring with tuneable Rashba spin-orbit interaction [3]. By propagating in segments it will be shown that Kramers-doublet qubits may be defined for which transformations on the Bloch sphere may be performed for an integral number of revolutions around the ring. The conditions for full coverage of the Bloch sphere will be determined and explained in terms of sequential qubit rotations due to electron motion along the segments, with change of rotation axes between segments due to adiabatic changes in the Rashba spin-orbit interaction. Prospects and challenges for possible realizations will be discussed for which rings based on InAs quantum wires are promising candidates [4].

[1] T. Cadez, J. H. Jefferson, and A. Ramsak, New J. Phys. 15, 013029 (2013).

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[3] A. Kregar, J. H. Jefferson, and A. Ramsak, arXiv:1511.06608.

[4] L. Ulcakar, A. Kregar, and A. Ramsak, to be submitted.

Random transverse-field Ising chain with long-range interactions

Róbert Juhász (Wigner Research Centre for Physics, Budapest, HUN) István A. Kovács (Center for Complex Networks Research and Department of Physics, Northeastern University, Boston, USA) Ferenc Iglói (Wigner Research Centre for Physics, Budapest, HUN)

Wednesday, February 17, 12:30-12:50

We study the low-energy properties of the long-range random transverse-field Ising chain with ferromagnetic interactions decaying as a power α of the distance. Using variants of the strong-disorder renormalization group method, the critical behavior is found to be controlled by a strong-disorder fixed point with a finite dynamical exponent $zc=\alpha$. Approaching the critical point, the correlation length diverges exponentially. In the critical point, the magnetization shows an α -independent logarithmic finite-size scaling and the entanglement entropy follows the area law. These observations are argued to hold even in higher dimensions. The same fixed point is expected to describe the critical behavior of an epidemic model, the random contact process with long-range spreading.

References

- 1. R. Juhász, I. A. Kovács, F. Iglói, Europhys. Lett., 107, 47008 (2014).
- 2. R. Juhász, I. A. Kovács, F. Iglói, Phys. Rev. E 91, 032815 (2015).

The associative nature of conference participation Jelena Smiljanic (Institute of Physics Belgrade, University of Belgrade, Belgrade, SRB) Marija Mitrovic Dankulov (Institute of Physics Belgrade, University of Belgrade, Belgrade, SRB)

Wednesday, February 17, 16:00-16:20

Patterns of scientific publications, collaborations and citations in scientific journals have been extensively studied in last decade while conference attendance patterns remain mostly unexplored from the perspective of statistical physics. In this work we study the conference participation at six national and international conferences of different sizes and from different fields of science. The gathered data contain detailed information about abstracts presented at the conferences for the period of 30 years, which enables us to analyse the total and successive number of participations, as well as the distribution of time lags between two successive participations for each author. All these properties exhibit truncated power-law behavior, regardless of the conference size and degree of specialization. This indicates that the probability for a scientist to reattend the specific conference is not constant, but rather it depends on the balance between the number of previous participations and non-participations. In order to further investigate the mechanism behind conference attendance patterns, we propose a microscopic stochastic model based on two key ingredients, 2-bin generalized Polya process and random termination time of a career. Using Monte Carlo simulations, we estimate the model parameters and demonstrate that this model, with positive feedback, can successively reproduce the empirically observed results. It is shown that an active participation in a conference series at the beginning strengthens the scientists association with that particular conference community and thus increases the probability of future participations. We expect to see similar participation patterns and dynamics in other types of social groups. In general, understanding mechanisms that underlie the repeated participation in the same conference series could have implications in social networks creation and optimization.

Posters

Poster abstract can be downloaded from the conference website

Monday 15, 14:00 - 15:20

1 Atamas, Nataliia

Percolation properties of hydrogen bond network in ionic liquids -non-polar substances solutions

2 Barash, Lev; Guskova, Maria ; Shchur, Lev

Program libraries PRAND and RNGAVXLIB for random number generation: employing parallelism of modern GPUs and CPUs

3 Barash, Lev; Borovsky, Michal; Weigel, Martin; Shchur, Lev

Improving and testing the population annealing algorithm

4 Beldowski, Piotr; Weber, Piotr; Peplowski, Piotr; Kruszewska, Natalia; Gadomski, Adam

Transporting hydrogen ions through structurally anisotropic, effectively one dimensional amphiphilic passages, as applied in terms of fractional dynamics

5 Bianchi, Emanuela

Heterogeneously Charged Colloids under confinement and in the bulk

6 Bittner, Elmar; Janke, Wolfhard

MuCa vs WL: A comparison

7 Cardelli, Chiara; Bianco, Valentino Coluzza, Ivan

Interplay between geometrical constrains and alphabet size in the design of patchy polymers

8 Chakraborty, Saikat; Das, Subir K.

Dynamics of Ordering in Ising Ferromagnets: Dependence upon initial correlation

9 Chalupa, Patrick; Kahl, Gerhard

Structural properties of a fluid of deformable spherical colloids

10 Chamati, Hassan; Romano, Silvano

Critical behaviour of some classical lattice spin models involving singular interactions

11 Corominas-Murtra, Bernat; Hanel, Rudolf; Thurner, Stefan

Sample Space Reducing processes and Targeted diffusion in complex networks: Universality in Scaling

12 Cristea, Artur

Lattice Boltzmann simulation of morfogenesys in bioprinted tissue-constuctructs

13 Dobnikar, Jure; Curk, Tine; Frenkel, Daan

Rational Design of Molecularly Imprinted Polymers

14 Dobnikar, Jure; Curk, Tine ; Frenkel, Daan

Nanoparticle Organization in Polymer Layers

15 Dobush, Oksana; Kozlovskii, Mykhailo

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16 Dolgushev, Maxim; Guérin, Thomas Blumen, Alexander; Bénichou, Olivier Voituriez, Raphaél

Contact Kinetics in Fractal Macromolecules

17 Domanski, Tadeusz

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18 Dudka, Maxym; Bénichou, Olivier ; Oshanin, Gleb ; Dietrich, Siegfried

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19 Eisler, Viktor; Zimborás, Zoltán

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20 Fabian, Balazs; Darvas, Maria ; Picaud, Sylvain ; Sega, Marcello ; Jedlovszky, Pal

The effect of anaesthetics on the properties of a lipid membrane in the biologically relevant phase: a computer simulation study

21 Falasco, Gianmaria; Baldovin, Fulvio ; Kroy, Klaus ; Baiesi, Marco

Mesoscopic virial equation for nonequilibrium statistical mechanics

22 Falasco, Gianmaria; Baiesi, Marco

Temperature response in nonequilibrium stochastic systems

23 Ferrari, Silvano; Bianchi, Emanuela ; Kahl, Gerhard

Hybrid crystal-liquid phase in inverse patchy colloids

24 Fomin, Yuriy; Ryzhov, Valentin; Tsiok, Elena; Brazhkin, Vadim; Trachenko, Kostya

Direct evidence for strong crossover of collective excitations and positive sound dispersion in the supercritical state of fluids

25 Gómez-Estévez, Juan Luis

McMillan-Mayer Solution Theory in a Semigrand Isothermal-Isochoric Ensemble

26 Gorev, Vyacheslav; Sokolovsky, Alexander

Non-linear relaxation in a spatially uniform plasma at the end of the relaxation processes

27 Hafner, Jonas; Rieger, Heiko

Quantum relaxation of the transverse Ising model

28 Halun, Joanna; Usatenko, Zoryana

Phantom ideal ring polymer chains in a slit geometry

29 Hucht, Fred

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30 Igloi, Ferenc; Kovacs, Istvan

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2 Leitão, Jorge; Lopes, J. M. Viana Parente ; Altmann, Eduardo G.

Monte Carlo Sampling in Chaotic Systems

3 Leitold, Christian; Dellago, Christoph

Nucleation and growth of cluster crystals

4 Lemmens, Lucien

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5 Léonard, Frédéric

Critical Exponents Can Be Different on the Two Sides of a Transition: A Generic Mechanism

6 Locatelli, Emanuele; Likos, Christos

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7 Mahnke, Reinhard

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53 Karner, Carina; Dellago, Christoph

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