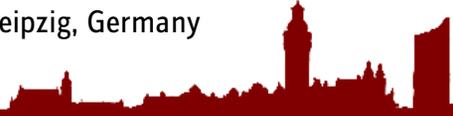


# MECO34

34th Conference of the Middle European Cooperation  
in Statistical Physics

30 March - 01 April 2009, Universität Leipzig, Germany



# BOOK OF ABSTRACTS

**600 JAHRE**

UNIVERSITÄT LEIPZIG





## Preface

The MECO conference series of the Middle European Cooperation in Statistical Physics was established under the leadership of Professor Alex Müller (Switzerland) in 1974. Originally the intention was to concentrate the activities on phase transitions and critical phenomena. Further the conference aimed at bringing together physicists from East- and West-European countries.

Traditionally, the MECO conferences run for three full days. The program is devoted to about 10 longer presentations or review talks by invited plenary speakers and about 20 shorter, more specialized contributed talks. All other participants are invited to present their recent research work on posters in order to avoid parallel sessions. The objective of the conference is to bring together renowned world-wide experts in the field of statistical physics.

The 34th MECO conference in Leipzig from 30 March to 1 April 2009 is planned to continue this tradition. On the one hand, the organizers intend to represent the most recent developments in many-body systems in such standard fields as the theory of phase transitions in equilibrium and non-equilibrium systems as well as of soft-matter materials, strongly correlated systems, transport in mesoscopic systems as well as biophysical problems.

Following the line of MECO, it is planned to review those achievements which were motivated and stimulated by earlier MECO conferences. Among them are, for instance, the application of renormalization group methods, the many Monte Carlo techniques which are based on and related to the statistical mechanics or the development of new successful methods for stochastic systems. Although the conference is dominated by theoretical methods, it is the expressly intention of the organizers to open the conference also for current experimental results presented by experimentalists.

Finally, we gratefully acknowledge generous financial support for the conference from the German Research Foundation (DFG), the Saxonian Ministry for Sciences and Arts (SMWK), the Wilhelm and Else Heraeus Foundation, the Deutsch-Französische Hochschule and the Springer-Verlag.

In the year of its 600th anniversary, we are warmly welcoming you at the University of Leipzig and look forward to an interesting and fruitful conference.

Wolfhard Janke (University of Leipzig, Germany)

Steffen Trimper (University of Halle, Germany)



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600 JAHRE  
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# MECO34

34th Conference of the Middle European Cooperation  
in Statistical Physics

30 March - 01 April 2009, Universität Leipzig, Germany



## Main Topics:

- Soft-matter physics
- Magnetic systems
- Complex systems and networks
- Non-equilibrium systems
- Interdisciplinary applications

## Organizers:

- Wolfhard Janke (Leipzig)
- Steffen Trimper (Halle)

## Invited Speakers:

- |                 |                         |
|-----------------|-------------------------|
| Günter Ahlers   | UC Santa Barbara, USA   |
| Hagen Kleinert  | FU Berlin, Germany      |
| David P. Landau | Univ. of Georgia, USA   |
| Hartmut Löwen   | Düsseldorf, Germany     |
| Georg Maret     | Konstanz, Germany       |
| Zoltán Rácz     | Budapest, Hungary       |
| Sidney Redner   | Boston Univ., USA       |
| Matthias Troyer | ETH Zürich, Switzerland |
| Royce Zia       | Virginia Tech, USA      |

<http://www.physik.uni-leipzig.de/~meco34>  
[meco34@itp.uni-leipzig.de](mailto:meco34@itp.uni-leipzig.de)



## Previous MECO Conferences

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

## International Advisory Board

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## Conference Schedule

**Monday, 30 March**

**08:50-09:00** WELCOME

### NON-EQUILIBRIUM PHYSICS

**09:00-09:40** Royce K. P. Zia Non-equilibrium statistical mechanics: A growing frontier of „pure and applied“ theoretical physics

**09:40-10:00** Viatcheslav Belyi Fluctuations out of equilibrium

**10:00-10:20** Karel Netočný Two approaches to dynamical fluctuations in small non-equilibrium systems

**10:20-10:40** Flemming Topsøe Interaction between truth, belief and knowledge as the key to entropy measures of statistical physics

**10:40-11:10** COFFEE

### COLLOIDAL SYSTEMS

**11:10-11:50** Georg Maret Melting and glass-transition of a 2D colloidal model system

**11:50-12:10** Juan R. Gomez-Solano Experimental verification of a modified fluctuation-dissipation relation for a colloidal particle in a non-equilibrium steady state

**12:10-12:30** Thomas Franosch Cluster-resolved dynamic scaling theory and universal corrections for transport on percolating systems

**12:30-14:00** LUNCH “Bayerischer Bahnhof”

**14:00-15:30** POSTER SESSION

### SOFT-MATTER SYSTEMS

**15:30-16:10** Hartmut Löwen Colloidal suspensions subjected to external fields

**16:10-16:30** Giancarlo Jug Why are window-glasses sensitive to magnetic fields at low temperatures?

**16:30-16:50** Hsiao-Ping Hsu Monte Carlo simulations of bottle-brush polymers in a good solvent

**16:50-17:20** COFFEE

### NETWORKS

**17:20-18:00** Sidney Redner Dynamical approach for solving complex networks

**18:00-18:20** Franco Maria Neri Stochastic epidemic processes on lattices: The role of heterogeneity

**18:20-18:40** Martin Bock Generalized Voronoi tessellation as a model of two-dimensional cell tissue dynamics

**20:00** DINNER “Thüringer Hof”

<b>Tuesday, 31 March</b>		
<b>CLASSICAL SIMULATIONS</b>		
<b>09:00-09:40</b>	David P. Landau	Monte Carlo simulations of systems with complex energy landscapes
<b>09:40-10:00</b>	Alexander Hartmann	New approaches to measuring ultrametricity and clustering of states
<b>10:00-10:20</b>	Fabien Paillusson	Modelling of the DNA-protein interaction
<b>10:20-10:40</b>	Alessandro Vindigni	Cross-over of universality class in the Ising chain frustrated by long-range interactions
<b>10:40-11:10</b>	<b>COFFEE</b>	
<b>STRUCTURE FORMATION</b>		
<b>11:10-11:50</b>	Günter Ahlers	Stochastically driven large-scale circulation in turbulent Rayleigh-Bénard convection
<b>11:50-12:10</b>	Reinhard Folk	Biconical critical dynamics
<b>12:10-12:30</b>	<b>ADVISORY BOARD MEETING</b>	
<b>12:30-14:00</b>	<b>LUNCH "Bayerischer Bahnhof"</b>	
<b>14:00</b>	<b>EXCURSION TO LUTHERSTADT-WITTENBERG/CONFERENCE DINNER</b>	

<b>Wednesday, 01 April</b>		
<b>QUANTUM SYSTEMS</b>		
<b>09:00-09:40</b>	Matthias Troyer	Continuous time QMC solvers for quantum impurity problems
<b>09:40-10:00</b>	Fabio Cinti	Phase transitions and magnetic orders in rare-earth Holmium ultra-thin films
<b>10:00-10:20</b>	Sandro Wenzel	Evidence for an unconventional universality class from a two-dimensional dimerized quantum Heisenberg model
<b>10:20-10:40</b>	Bertrand Berche	Gauge field theory approach to spin transport in 2D electron gas
<b>10:40-11:10</b>	<b>COFFEE</b>	
<b>DISORDERED SYSTEMS</b>		
<b>11:10-11:30</b>	Thomas Nattermann	Localized states and interaction induced delocalization in Bose gases with quenched disorder
<b>11:30-11:50</b>	Francesco Parisen Toldin	Strong-disorder paramagnetic-ferromagnetic fixed point in the square-lattice $\pm J$ Ising model
<b>11:50-12:10</b>	Ralph Kenna	The site-diluted Ising model in two and four dimensions
<b>12:10-12:30</b>	Hans Fogedby	Patterns in the KPZ equation: Mapping of a stochastic equation to Hamilton equations of motion in the weak noise limit
<b>12:30-14:00</b>	<b>LUNCH "Bayerischer Bahnhof"</b>	
<b>14:00-15:30</b>	<b>POSTER SESSION</b>	
<b>DYNAMICAL PROCESSES</b>		
<b>15:30-16:10</b>	Zoltan Rácz	Controlling precipitation patterns through electric currents
<b>16:10-16:30</b>	Paolo Politi	A coalescing particles system arising from the conserved Kuramoto-Sivashinsky equation
<b>16:30-16:50</b>	Zoryana Usatenko	The monomer density profiles across the slit: Massive field theory approach
<b>16:50-17:20</b>	<b>COFFEE</b>	
<b>FIELD THEORY</b>		
<b>17:20-18:00</b>	Hagen Kleinert	Multivalued Fields
<b>18:00-18:10</b>	<b>CLOSING</b>	
<b>20:00</b>	<b>DINNER (jointly with BuildMoNa-Symposium) "Thüringer Hof"</b>	



## Abstracts of Invited Talks

## 1.1 Stochastically driven large-scale circulation in turbulent Rayleigh-Bénard convection

Günter Ahlers

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A major component of the dynamics of turbulent Rayleigh-Bénard convection (RBC) in a fluid heated from below is a large-scale circulation (LSC). For cylindrical geometries with the height  $L$  close to the diameter  $D$  the LSC consists of a single convection roll, with both down-flow and up-flow near the side wall but at azimuthal locations  $\theta_0$  that differ by  $\pi$ . First this talk will present experimental results for the dynamics of the LSC in cylindrical samples of aspect ratio  $\Gamma \equiv D/L \simeq 1$ . Then these data will be compared with results from a theoretical Navier-Stokes (NS) motivated model of the LSC that consists of two coupled stochastic ordinary differential equations. In this model the stochastic terms represent the driving of the LSC by the small-scale turbulent fluctuations.

An interesting aspect of the LSC dynamics is a lateral twisting oscillation on a relatively fast time scale of the (on average) near-vertical circulation plane. The azimuthal displacement of this mode has a Gaussian probability distribution, consistent with a stochastically driven damped oscillator. On a longer time scale the orientation  $\theta_0$  of the circulation plane, under the influence of the turbulent background fluctuations, undergoes azimuthal diffusion. Another important feature consists of rare relatively fast re-orientation events of  $\theta_0$  due to cessations of the flow. The angular change during cessations has a uniform probability distribution  $p(\Delta\theta)$ , and cessations have a Poisson distribution in time.

The second part of this talk will discuss various perturbations that break the rotational invariance of the cylindrical system. One of these is due to Earth's Coriolis force which leads to a  $p(\theta_0)$  that has a maximum in a westerly direction. This result is reproduced quantitatively by a Fokker-Planck equation based on the model potential and the measured azimuthal diffusivity. Another perturbation that will be examined theoretically is a slight departure from a circular horizontal cross section, such as an elliptical distortion of the sample. A further perturbation under consideration is the influence of a slight tilt of the cylinder axis relative to gravity. Both an elliptic cross section and a tilt lead to a new stochastically driven oscillatory mode that differs from the torsional mode already present in the perfect system

by being uniform along the height of the sample. In the tilted case experimental measurements of this mode will be discussed. We show that certain perturbations, such as the Coriolis force and an elliptic cross section, influence only the orientation and not the amplitude of the LSC; these are predicted not to affect the frequency of cessations. Other perturbations, such as a tilt, affect both the orientation and the amplitude of the flow and strongly suppress cessations.

[1] E. Brown and G. Ahlers, arXiv:0902.4487 (2009).

## I.2 Multivalued fields

**Hagen Kleinert**

Institut für Theoretische Physik, FU Berlin, Arnimallee 14,  
D-14195 Berlin, Germany  
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We show how to employ multivalued fields to understand the statistical properties of line-like vortices, defects, and geometries, and their phase transitions.

## I.3 Monte Carlo simulations of systems with complex energy landscapes

**David P. Landau**

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Systems with complex energy landscapes are common in nature and present particular problems for standard Monte Carlo algorithms because of the long time scales that result at low temperatures where interesting behavior occurs. Several methods have been devised for such cases, and we shall describe a simple, iterative approach, termed Wang-Landau sampling [1] in the literature, that is extremely effective for diverse types of systems. After presenting the algorithm we shall demonstrate its effectiveness for a simple spin glass model. Then, we shall introduce a minimalistic hydrophobic/hydrophilic (HP) lattice protein model and present results for both ground states (native states) and thermodynamic properties for several such proteins.

Lastly, we shall describe a study of a realistic membrane protein model. Together, these results demonstrate advances in our understanding of the behavior of diverse systems at the intersection between statistical physics and biology, all of which possess rough energy landscapes [2].

[1] F. G. Wang and D. P. Landau, Phys. Rev. Lett. **86** (2001) 2050.

[2] T. Wuest, D. P. Landau, C. Gervais, and Y. Xu., Comp. Phys. Comm. (in press).

## **I.4 Colloidal suspensions subjected to external fields**

**Hartmut Löwen**

Institut für Theoretische Physik II, University of Düsseldorf, Universitätsstraße 1,  
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Dispersions of colloidal particles are excellent model systems of classical statistical mechanics in order to understand the principles of self-organization processes. Using an external field (e.g. electric or magnetic field) the effective interaction between the colloidal particles can be tailored and the system can be brought into non-equilibrium in a controlled way. Partial clustering and crystallization in two-dimensional superparamagnetic binary colloidal mixtures will be discussed as well as lane formation in mixtures of charged suspensions driven by an electric field.

## **I.5 Melting and glass-transition of a 2D colloidal model system**

**Georg Maret**

Dept. of Physics, University of Konstanz, D-78457 Konstanz, Germany  
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Micron sized colloidal particles in suspension are ideal model systems to study structural and dynamic properties of condensed matter at atomic scales because, unlike atoms, colloidal particle motions can be conveniently tracked on all relevant time and length scales by video-microscopy and inter-particle interactions are widely tun-

able. This will be illustrated by exploiting a 2D system of superparamagnetic colloids which are pinned at the flat air/water interface and interact with  $1/r^3$  dipole-dipole pair potential tuned by an external magnetic field [1].

Using monodisperse particles the system forms large hexagonal crystals and we find [2] full quantitative evidence for the two-step melting scenario according to the prediction of KTHNY [3]. Fluctuations of particle positions allow to determine phonon dispersion relations and elastic constants of the crystals [4]. The latter control the appearance of thermally excited topological defects, in particular those involved in 2D melting. Binary mixtures form 2D glasses [5] with pronounced frustration of local crystalline order, partial clustering and heterogeneous dynamics [6].

- [1] F. Ebert *et al.*, arXiv:0903.2808 (2009).
- [2] H. H. von Grünberg, P. Keim, and G. Maret, Phase transitions in two-dimensional colloidal systems. In: G. Gompper and M. Schick, Eds., *Soft Matter*, Vol. 3: Colloidal Order: Entropic and Surface Forces (Wiley-VCH Verlag, Weinheim, 2007), pp. 41-85.
- [3] J. M. Kosterlitz and D. J. Thouless, *J. Phys. C* **6** (1973) 1181; A. P. Young, *Phys. Rev. B* **19** (1979) 1855; D. R. Nelson and B. I. Halperin, *Phys. Rev. B* **19** (1979) 2457.
- [4] P. Keim, G. Maret, U. Herz, and H. H. von Grünberg, *Phys. Rev. Lett.* **92** (2004) 215504; P. Keim, G. Maret, and H. H. von Grünberg, *Phys. Rev. E* **75** (2007) 031402.
- [5] H. König *et al.*, *Eur. Phys. J. E* **18** (2005) 287; M. Bayer *et al.*, *Phys. Rev. E* **76** (2007) 011508.
- [6] F. Ebert, P. Keim, and G. Maret, *Eur. Phys. J. E* **26** (2008) 161; N. Hoffmann *et al.*, *Phys. Rev. Lett.* **97** (2006) 078301.

## I.6 Controlling precipitation patterns through electric currents

**Ioana Bena<sup>1</sup>, Michel Droz<sup>1</sup>, István Lagzi<sup>2</sup>, Kirsten Martens<sup>1</sup>,  
Zoltan Rácz<sup>3</sup>, Andreas Volford<sup>4</sup>**

<sup>1</sup>Theoretical Physics Department, University of Geneva, Switzerland

<sup>2</sup>Institute of Chemistry, Eötvös University, Budapest, Hungary

<sup>3</sup>Institute for Theoretical Physics, Eötvös University,  
Pazmany s. 1/a, H-1117 Budapest, Hungary

<sup>4</sup>Department of Physics, University of Technology and Economics,  
Budapest, Hungary  
`racz@general.elte.hu`

Understanding and controlling precipitation patterns emerging in reaction-diffusion processes is of fundamental importance with high potential for technical applications. Here we present a theory showing that precipitation resulting from reactions among charged agents can be controlled by an appropriately designed, time-dependent electric current. Examples of current dynamics yielding periodic bands of prescribed wavelength, as well as more complicated structures are given. The pattern control is demonstrated experimentally on the reaction-diffusion-precipitation process  $2\text{AgNO}_3 + \text{K}_2\text{Cr}_2\text{O}_7 \rightarrow \underline{\text{Ag}_2\text{Cr}_2\text{O}_7} + 2\text{KNO}_3$  taking place in a gel.

## I.7 Dynamical approach for solving complex networks

**Sidney Redner**

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The master equation approach is applied to quantify the structure of complex growing networks. First, the degree distribution and the nature of the percolation transition are derived for the classical Erdős-Renyi random graph. For the random recursive tree, the degree distribution and the network diameter are obtained by the master equation. It is also shown that augmenting the growth mechanism of the random recursive tree by “redirection” leads to linear preferential attachment. Finally, the universality classes of networks that grow by preferential attachment are outlined. Linear preferential attachment gives a power-law degree distribution, but the as-

sociated exponent sensitively depends on microscopic model details. For sublinear attachment rates a robust stretched exponential degree distribution arises, while for superlinear attachment singular behavior arises in which a single node is linked to nearly every other node in the network.

## **I.8 Continuous time QMC solvers for quantum impurity problems**

**Matthias Troyer**

Theoretische Physik, ETH Zürich, CH-8093 Zürich, Switzerland  
troyer@phys.ethz.ch

Dynamical mean field calculations involve the repeated numerical solution of an impurity problem, which is the time critical step in the self-consistency loop. The performance and flexibility of available impurity solvers therefore defines what type of problems can be treated within dynamical mean field theory. Over the past few years, significant progress has been achieved with the development of continuous-time quantum Monte Carlo methods. These algorithms are based on a diagrammatic expansion of the partition function in either the interactions or hybridizations, and the stochastic sampling of appropriate collections of diagrams. I will explain the key ideas behind this powerful and versatile approach, and will give an outlook over what problems can be solved by these new methods.

## **I.9 Non-equilibrium statistical mechanics: A growing frontier of “pure and applied” theoretical physics**

**R. K. P. Zia**

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rkpzia@vt.edu

Founded over a century ago, statistical mechanics for systems in thermal equilibrium has been so successful that, nowadays, it forms part of our physics core curriculum. On the other hand, most of “real life” phenomena occur under non-equilibrium con-

ditions. Unfortunately, statistical mechanics for such systems is far from being well established. The goal of understanding how complex macroscopic behavior emerge from simple microscopic rules (of evolution, say) remains elusive. As an example of the difficulties we face, imagine trying to predict the existence of a tree from a collection of H, C, O, N, ... atoms, evolving according to the rules of EM and QM.

Over the last three decades, an increasing number of condensed matter theorists are devoting their efforts to this frontier. After a brief summary of the crucial differences between equilibrium and non-equilibrium statistical mechanics, I will give a bird's-eye view of some key issues, ranging from the "fundamental" to (a small set of) the "applied". The methods used also span a wide spectrum, from "easy" computer simulations to sophisticated field theoretic techniques. These will be illustrated in the context of some recent on-going projects [1] at Virginia Tech.

[1] R. K. P. Zia and B. Schmittmann, JSTAT (2007) P07012.



## Abstracts of Contributed Talks

### C.1 Fluctuations out of equilibrium

**Viatcheslav Belyi**

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Fluctuations play an important role in the constitution of dissipative structures [1, 2], in the sensitivity of the devices and find applications in diagnostic procedures. In thermodynamic equilibrium, the fluctuations are determined by the system temperature and the dissipation [3]. The matter becomes more delicate even in the local-equilibrium case. In the general case parameters of the systems can be change in both time and space. Inhomogeneities in space and time of these quantities will certainly also contribute to the fluctuations. In the context of plasma physics, using the Langevin approach and the time-space multiscale technique, it has been shown that the amplitude and the width of the spectral lines of the electrostatic field fluctuations and the electron form factor are determined not only by the imaginary (dissipative) part of the dielectric susceptibility but also by the derivatives of its real (dispersive) part [4]. As a result of the inhomogeneity, these properties become asymmetric with respect to the inversion of the sign of the frequency. In the kinetic regime, the form factor is more sensitive to space gradients than the spectral function of the electrostatic field fluctuations. This asymmetry of lines can be used as a diagnostic tool to measure local gradients in the plasma. The fluctuation-dissipation relation has been generalized to the non-equilibrium systems with slowly varying parameters [5]. The important conclusion of this analysis is to reveal that the spectral function of the fluctuations is determined not only by dissipation but also by the derivatives of the dispersion. The non-Joule dispersion contribution is characterized by a new non-local effect originating from an additional phase shift between the force and the response of the system. That phase shift results from the parametric control to the system. The example of an electrical oscillation circuit shows the dispersive contributions strongly affect the quality factor. These results are applicable to other systems and are important for the understanding of various behaviors observed in different field of physics.

- [1] G. Nicolis and I. Prigogine, *Nonequilibrium Systems. From Dissipative Structure to Order Through Fluctuations* (Wiley, New York, 1979).
- [2] W. Horsthemke and R. Lefever, *Noise-Induced Transitions* (Springer-Verlag, Berlin, 1984).
- [3] H. B. Callen and T. A. Welton, *Phys. Rev.* **83** (1951) 34.
- [4] V. V. Belyi, *Phys. Rev. Lett.* **88** (2002) 255001.
- [5] V. V. Belyi, *Phys. Rev. E* **69** (2004) 017104.

## **C.2 Gauge field theory approach to spin transport in 2D electron gas**

**Bertrand Berche**

Statistical Physics Group, IJL, Nancy University, F-54506 Vandoeuvre, France  
berche@lpm.u-nancy.fr

We discuss the Pauli Hamiltonian within a  $SU(2)$  gauge theory interpretation, where the gauge symmetry is broken. This interpretation carries directly over to the structural inversion asymmetric spin-orbit interactions in semiconductors and offers new insight into the problem of spin currents in the condensed matter environment. The central result is that symmetry breaking leads to zero spin conductivity in contrast to predictions of Gauge symmetric treatments. Computing the translation operator commutation relations comprising the simplest possible structural inversion asymmetry due to an external electric field, we derive a new condition for orbit quantization. The relation between the topological nature of this effect is consistent with our non-Abelian gauge symmetry breaking scenario.

- [1] E. Medina, A. López, and B. Berche, *Europhys. Lett.* **83** (2008) 47005.

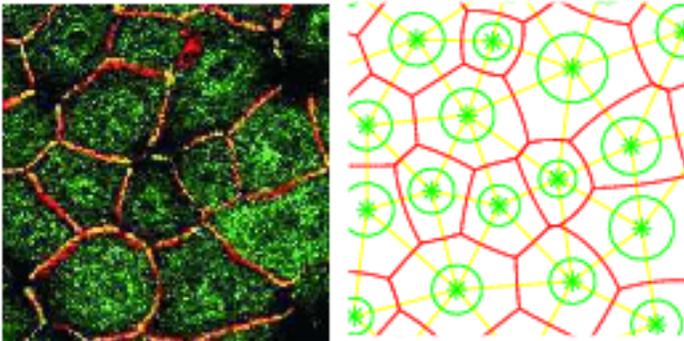
## C.3 Generalized Voronoi tessellation as a model of two-dimensional cell tissue dynamics

**Martin Bock**

IZMB, Universität Bonn, Kirschallee 1–3, D-53115 Bonn, Germany  
mab@uni-bonn.de

Voronoi tessellations have been used to model the geometric arrangement of cells in biological tissues, however so far only with flat hypersurfaces as cell-cell contact borders. In order to reproduce the experimentally observed piecewise spherical boundary shapes, we develop a consistent theoretical framework of multiplicatively weighted distance functions, defining generalized finite Voronoi neighborhoods around cell bodies of varying radius, which serve as heterogeneous generators of the resulting model tissue. The interactions between cells are represented by adhesive and repelling force densities on the cell contact borders. Moreover, protrusive locomotion forces are implemented along the cell boundaries at the tissue margin, and stochastic perturbations allow for non-deterministic motility effects. MD-type simulations of the emerging system of stochastic differential equations for position and velocity of cell centers show the feasibility of this Voronoi method generating realistic cell shapes. Finally an argument is derived pointing to a tradeoff in natural tissues between cell size heterogeneity and the extension of cellular lamellae.

[1] M. Bock, A. K. Tyagi, J.-U. Kreft, and W. Alt, arXiv:0901.4469 (2009).



Typical microscopic picture of an epithelial monolayer (left) and simulated cell tissue (right).

## C.4 Phase transitions and magnetic orders in rare-earth Holmium ultra-thin films

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In the last decades, a large effort has been devoted to the study of low dimensional frustrated magnetic systems, where a non-collinear order, characterized by a possibly large modulation, is established.

Some rare-earth elements (as Holmium, Dysprosium or Terbium) and their compounds are typical examples that the nature makes available to investigate such peculiar behaviors, in view of the variety of magnetic arrangements, as helix, spiral or longitudinal-wave, that can be observed in bulk samples of such materials [1]. Further examples of helicoidal structures can also be met in multiferroic materials and itinerant systems.

In magnetic systems with frustration, the lack of translational invariance due to the presence of surfaces can result especially important for ultra-thin film samples, where the thickness is comparable, or even lower, with the wave length of the ordered magnetic structure observed in the bulk. Many fundamental features related to such systems have not yet been exhaustively investigated and completely understood, and ultra-thin films of rare-earth elements are still among the most intriguing layered systems to be studied[2, 3].

In order to clarify some of the present issues, we have performed an extensive Monte Carlo simulation of films of different thickness, assuming different model Hamiltonians which correctly describe the rare-earth bulk magnetic behaviour. For low enough thicknesses the film properties are clearly affected by the strong competition among the helical pitch and the surface effects, which involve the majority of the spin layers. Under these conditions different magnetic phases emerge, with the high-temperature, disordered, paramagnetic phase and the low-temperature, long-range ordered one separated by an intriguing intermediate-temperature block phase, where outer ordered layers coexist with some inner, disordered ones. The phase transition of these inner layers displays the signatures of a Kosterlitz-Thouless one [4, 5].

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## C.5 Patterns in the KPZ equation: Mapping of a stochastic equation to Hamilton equations of motion in the weak noise limit

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A nonperturbative weak noise scheme is applied to the Kardar-Parisi-Zhang equation for a growing interface in all dimensions [1]. It is shown that the growth morphology can be interpreted in terms of a dynamically evolving texture of localized growth modes with superimposed diffusive modes. Applying Derrick's theorem it is conjectured that the upper critical dimension is four [2, 3].

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## C.6 Biconical critical dynamics

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Anisotropic antiferromagnets in an external field (in three spatial dimensions) are fascinating systems showing several phases of magnetic ordering separated by lines of continuous phase transitions meeting in a multicritical point. Renormalization group (RG) theory has recently shown that in general the biconical fixed point (related to a tetracritical point) is stable. Under special thermodynamic conditions the Heisenberg fixed point could be stable which then would lead to a bicritical point.

The dynamical critical behavior is especially rich. At the multicritical point two lines belonging to different universality classes meet. A new dynamical universality class (biconical dynamics) is governed by their meeting point (biconical fixed point).

At low values of the external magnetic field the dynamics near the transition from the paramagnetic to the antiferromagnetic phase belongs to the universality class of model C (relaxational dynamics of the order parameter coupled statically to a conserved density). At higher values of the external magnetic field the transition from the paramagnetic to the spin flop phase belongs to model F (relaxational dynamics of the order parameter coupled statically and dynamically to a conserved density).

Our results calculated within two loop order of RG theory bring about the presence of small static and even smaller dynamic slow transients. Therefore an effective critical behavior might be expected. The important advantage of this magnetic system is that the dynamical correlations of both the non conserved order parameter and the conserved density are in principle experimentally accessible by neutron scattering.

Acknowledgement: This work was supported by the Fonds zur Förderung der wissenschaftlichen Forschung under Project No. P19583-N20.

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## **C.7 Cluster-resolved dynamic scaling theory and universal corrections for transport on percolating systems**

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For a continuum percolation model, it has been shown recently that the crossover from pure subdiffusion to normal diffusion extends over five decades in time [1, 2]; in addition, the asymptotic behaviour is slowly approached and the large corrections cannot simply be ignored. Thus, it is of general interest to develop a systematic description of universal corrections to scaling in percolating systems.

For percolating systems, we propose a universal exponent relation connecting the leading corrections to scaling of the cluster size distribution with the dynamic

corrections to the asymptotic transport behaviour at criticality. Our derivation is based on a cluster-resolved scaling theory unifying the scaling of both the cluster size distribution and the dynamics of a random walker. We corroborate our theoretical approach by extensive simulations for a site percolating square lattice and numerically determine both the static and dynamic correction exponents [3].

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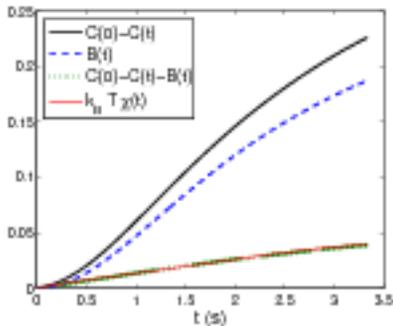
## **C.8 Experimental verification of a modified fluctuation-dissipation relation for a colloidal particle in a non-equilibrium steady state**

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A modified fluctuation-dissipation theorem (MFDT) has been recently found for simple Langevin dynamics close to non-equilibrium steady states (NESS) with non-vanishing probability currents [1]. In this work we verify experimentally MFDT for fluctuations of a micron-sized silica particle immersed in water moving in a periodic potential and subjected to a non-conservative constant force. A NESS is implemented by means of a toroidal optical trap created by a rotating laser beam with intensity modulation which confines the motion of the particle on a circle [2]. We measure the autocorrelation function  $C(t) = \langle O(\theta(t'))O(\theta(t' + t)) \rangle$  of an observable  $O$  related to the angular position  $\theta$  of the particle, the corresponding integrated response function  $\chi(t)$  due to a small perturbation of the amplitude of the periodic potential, and a corrective term  $B(t)$  given by the constant probability current of the particle. We verify the MFD relation  $C(0) - C(t) - B(t) = k_B T \chi(t)$ , as shown theoretically by [1] (see Figure). The validity of MFDT can be interpreted as a restoration of an equilibrium-like fluctuation-dissipation relation in the Lagrangian frame moving at the mean local velocity of the particle determined by the probability current.

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Comparison between the different terms involved in the MFDT as a function of the time lag  $t$ .

## C.9 New approaches to measuring ultrametricity and clustering of states

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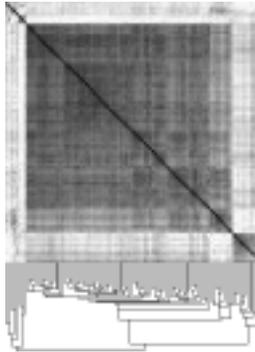
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We present results [1] from Monte Carlo simulations to test for ultrametricity (UM) and clustering properties in spin-glass models. For this purpose, we introduce a different normalization of an UM measure, which allows to distinguish real UM from the spurious UM of the paramagnetic phase, in contrast to previous approaches. Furthermore, we extend a hierarchical clustering approach [2], resulting in displaying the hierarchical organization of a set of configurations via a dendrogram and a grey scale picture of the matrix  $d_{\alpha\beta}$  of hamming distances (see figure). The extension allows to count the number of top-level clusters of the configuration space in a well-defined way. These approaches are applicable to a wide range of models in disordered systems, like spin glasses [3] or combinatorial optimization problems [4], which are well known for their complex configuration landscapes.

By using a one-dimensional Ising spin glass with random power-law interactions [5], where the universality class of the model can be tuned by changing the power-law exponent, we find signatures of UM behavior both in the mean-field and

non-mean-field universality classes for large linear system sizes. Furthermore, we confirm the existence of nontrivial connected components in phase space via a clustering analysis of configurations.

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A dendrogram obtained by clustering 100 configurations for a sample system with long-range interactions (SK model) and  $N = 512$  at  $T = 0.4$  together with the matrix  $d_{\alpha\beta}$  shown in grey scale (distance 0 is black). The order of the states is given by the leaves of the dendrogram (figure rotated clockwise by  $90^\circ$ ).

## C.10 Monte Carlo simulations of bottle-brush polymers in a good solvent

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Single bottle-brush polymers with a flexible backbone and flexible side chains are studied in a good solvent. They are simulated by using the bond fluctuation model

on a simple cubic lattice with Monte Carlo simulations. A coarse grained model for the special case of a rigid backbone is also used for comparison. Varying the side chain length, backbone length, and the grafting density, the scaling behavior of the radius of gyration, end-to-end distance, and the radial density profiles of monomers and side chain ends are estimated and checked with the previous theoretical predictions [1]. In order to compare our results with experimental scattering data, the structure factors describing the scattering from a single side chain and from the total bottle-brush polymer are also estimated. To describe effects due to the finiteness of the backbone, free ends of the backbone are considered in our simulations. The inhomogeneity of the structure in the direction along the backbone is carefully investigated. With our simulation results we test various phenomenological models that have been proposed to interpret experimental scattering data for bottle-brush polymers. A detailed analysis of radial density profile and the total scattering of a bottle-brush are given [2].

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## **C.11 Why are window-glasses sensitive to magnetic fields at low temperatures?**

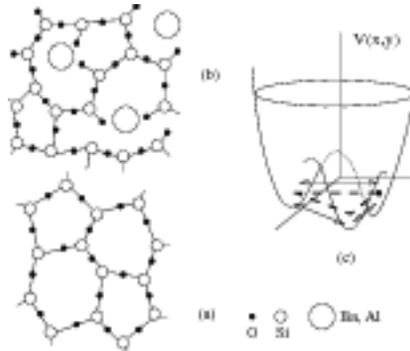
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Recent experiments on the thermal and dielectric properties of multicomponent silicate glasses at low temperatures ( $< 1$  K) have revealed an unusual response in some thick-film glass sensors to an applied magnetic field. The heat capacity, which should be linear with temperature, has a non-monotonic response to the field, the dielectric constant has both an enhancement peaking around 1000 Gauss and a suppression beginning around 2000 Gauss. Theories proposed so far, based on a mesoscopic coherent tunneling state or on a nuclear dipole/quadrupole coupling mechanism, have been unable to explain qualitatively most of the experimental findings. A statistical-mechanics theory will be presented which explains quantitatively all of these puzzling experimental findings. The theory is based on an extension of the standard tunneling model for structural low-temperature glasses in which the tunneling particles are assumed to move in a multi-welled local potential. The theory does explain the

thermomagnetic enhancement as well as both the magnetocapacitance enhancement and subsequent suppression. It turns out that a small cluster of coherently tunneling charged particles is involved in what are basically multicomponent, multiphase complex materials.

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## C.12 The site-diluted Ising model in two and four dimensions

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The Ising model with uncorrelated, quenched random-site or random-bond disorder has been controversial in both two and four dimensions. In these dimensions, the leading exponent  $\alpha$ , which characterizes the specific-heat critical behaviour, vanishes and no Harris prediction for the consequences of quenched disorder can be made. In the two-dimensional case, the controversy is between the strong universality hypothesis which maintains that the leading critical exponents remain the same as in the pure

case and the weak universality hypothesis, which favours dilution-dependent leading critical exponents. In the four-dimensional case unusual corrections to scaling characterize the model, and the precise nature of these corrections has been debated. Here both versions of the model are subject to finite-size scaling analyses, paying special attention to the implications for multiplicative logarithmic corrections. The analysis is fully supportive of the scaling relations for logarithmic corrections and of the strong scaling hypothesis in the 2D case. Progress is also made in determining the correct 4D scenario.

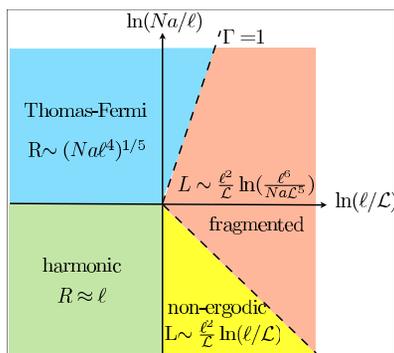
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## C.13 Localized states and interaction induced delocalization in Bose gases with quenched disorder

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Very diluted Bose gas placed into a disordered environment falls into a fragmented localized state. At some critical density the repulsion between particles overcomes the disorder. The gas transits into a coherent superfluid state. In this talk the geometrical and energetic characteristics of the localized state at zero temperature and the critical density at which the quantum phase transition from the localized to the superfluid state proceeds are found.



## C.14 Stochastic epidemic processes on lattices: The role of heterogeneity

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Stochastic epidemic processes of the SIR (susceptible-infected-recovered) type on lattices are well known to be equivalent to isotropic bond percolation by means of a simple mapping of parameters. However, when the system is heterogeneous, i.e. there is quenched disorder in host parameters, this mapping is no longer valid, and no unique parameter is known to describe the phase transition between invading and non-invading regimes in such systems. By numerical study of epidemics with several different distributions for disorder, we found evidence that the position of the threshold for invasion can be accounted for by the first two moments of the distribution, higher moments giving just small corrections. We show how these results can be exploited to control disease spreading on heterogeneous systems.

## C.15 Two approaches to dynamical fluctuations in small non-equilibrium systems

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Within the framework of Markov [1, 2, 3, 4] and Semi-Markov [5] processes modeling a small nonequilibrium system, we discuss two complementary approaches to the long-time asymptotics of dynamical fluctuations.

The first approach is a variant of the Onsager-Machlup theory suitable for mesoscopic systems, using a decomposition of the fluctuations into the time-symmetric

(occupations) and the time-antisymmetric (currents) sectors. We give an explicit form of the Onsager-Machlup Lagrangian in terms of the entropy production and the dynamical activity, [1, 2, 3, 5]. This formulation identifies ‘natural’ dynamical observables and provides variational formulas for derived fluctuation functionals. It is also suitable for discussing the status of variational principles based on the entropy production.

The second approach is based on the perturbative computation of the generating functions, using the Feynman-Kac representation and the Rayleigh-Schrödinger scheme, [4]. This formulation enables a numerically exact calculation of, e.g., current cumulants to high order.

Both approaches will be discussed and compared.

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## C.16 Modelling of the DNA-protein interaction

**Fabien Paillusson<sup>1</sup>, Maria Barbi<sup>1</sup>, Jean-Marc Victor<sup>1</sup>,  
Vincent Dahirel<sup>2</sup>, Marie Jardat<sup>2</sup>**

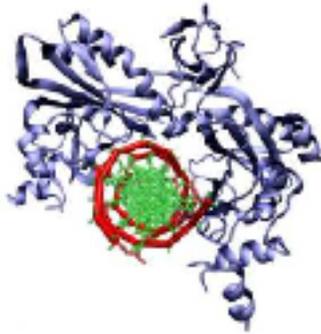
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The structure of DNA Binding Proteins enables a strong interaction with their specific target site on DNA. However, recent single molecule experiment reported that proteins can diffuse on DNA. This suggests that the interactions between proteins and DNA play a role during the target search even far from the specific site. It is unclear how these non-specific interactions optimize the search process, and how the protein structure comes into play. Each nucleotide being negatively charged, one may think that the positive surface of DNA-BPs should electrostatically collapse onto DNA. Here we show by means of Monte Carlo simulations and analytical calculations that a counter-intuitive repulsion between the two oppositely charged macromolecules exists at a nanometer range. We also show that this repulsion is due to a local increase of the osmotic pressure exerted by the ions which are trapped at the interface. For the concave shape of DNA-BPs, and for realistic protein charge

densities, we find that the repulsion pushes the protein in a free energy minimum at a distance from DNA. As a consequence, a favorable path exists along which proteins can slide without interacting with the DNA bases. When a protein encounters its target, the osmotic barrier is completely counter-balanced by the H-bond interaction, thus enabling the sequence recognition.

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## C.17 Strong-disorder paramagnetic-ferromagnetic fixed point in the square-lattice $\pm J$ Ising model

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We consider the random-bond  $\pm J$  Ising model on a square lattice as a function of the temperature  $T$  and of the disorder parameter  $p$  ( $p = 1$  corresponds to the pure Ising

model). We investigate the critical behavior along the paramagnetic-ferromagnetic transition line at low temperatures, below the temperature of the multicritical Nishimori point at  $T^* = 0.9527(1)$ ,  $p^* = 0.89083(3)$ . We present finite-size scaling analyses of Monte Carlo results at two temperature values,  $T \approx 0.645$  and  $T = 0.5$ . The results show that the paramagnetic-ferromagnetic transition line is reentrant for  $T < T^*$ , that the transitions are continuous and controlled by a strong-disorder fixed point with critical exponents  $\nu = 1.50(4)$ ,  $\eta = 0.128(8)$ , and  $\beta = 0.095(5)$ . This fixed point is definitely different from the Ising fixed point controlling the paramagnetic-ferromagnetic transitions for  $T > T^*$ . Our results for the critical exponents are consistent with the hyperscaling relation  $2\beta/\nu - \eta = d - 2 = 0$ .

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## C.18 A coalescing particles system arising from the conserved Kuramoto-Sivashinsky equation

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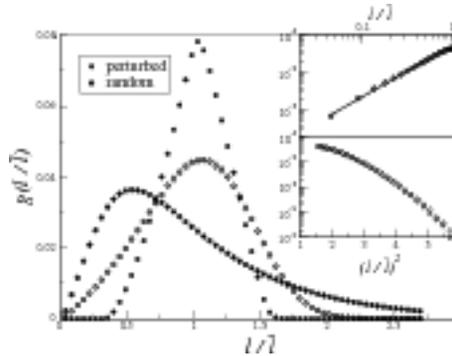
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We study an interacting particles system arising from a mapping to the conserved Kuramoto-Sivashinsky equation,  $u_t = -(u + u_{xx} + u_x^2)_{xx}$ , which appears in crystal growth and sand-ripple dynamics. Particles represent vanishing regions of diverging curvature, joined by arcs of a universal parabola; nearest particles are attracted to one another at a rate inversely proportional to their distance, and coalesce upon encounter.

The growing interparticle distance  $\ell$  represents coarsening of the system, and we are able to establish the scaling  $\ell(t) \sim \sqrt{t}$ . We obtain its probability distribution function,  $g(\ell)$ , numerically, and study it analytically within the hypothesis of uncorrelated intervals, finding a non-trivial power-law at small distances, and a faster than gaussian decay at large distances.

At yet an higher level of abstraction, trails of coalescing events may too be viewed as *particles* that propagate ballistically at a speed proportional to the background density, and that annihilate upon encounter.

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The asymptotic distribution of interparticle distances (empty symbols) for two different initial distributions (full symbols): random (diamonds) distribution and slightly perturbed (circles) uniform distribution. The system length is  $L = 10^6$  and there are  $10^5$  particles at the beginning. The asymptotic distribution is shown at time  $t = 10^5$ , and is averaged over hundreds of runs. Upper inset:  $g(\ell/\bar{\ell})$  at small distances, on a log-log scale. Lower inset:  $g(\ell/\bar{\ell})$  vs.  $(\ell/\bar{\ell})^2$  at large distances, on a lin-log scale.

## C.19 Interaction between truth, belief and knowledge as the key to entropy measures of statistical physics

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It is our goal to isolate the truly important notions of entropy for statistical physics. Until not that long ago, the one and only notion, *classical entropy*, was the one rooted in works of Boltzmann and Gibbs and consistent with the later theory developed by Shannon. A multitude of other notions have been suggested by mathematicians since the fifties and in 1971 the first suggestion of new entropies for use in statistical physics were published by Lindhard and Nielsen. This was met with little interest. It was not until 1988 when Tsallis, unaware of previous research, pointed to the same entropy measures that had appeared in the paper by Lindhard and Nielsen (and in earlier mathematical literature) that the development gained momentum. Since then more than 2500 publications have studied the entropies now bearing Tsallis'

name and also referred to as  $q$ -entropies with  $q$  a real parameter. Classical entropy is obtained when  $q = 1$ .

Tsallis' success in promoting the  $q$ -entropies seems to be due to his direct and pragmatic approach, as well as to the demonstration by Tsallis and followers that for a long list of phenomena,  $q$ -entropies lead to a better match with data than classical entropy. As another attractive feature, note that when applying Jaynes *maximum entropy principle* with  $q$ -entropy in place of classical entropy, then, typically, power laws result from the analysis. These laws (distributions) were, and still are, popular because of their scale invariance and heavy-tail behaviour.

In spite of the attraction to many, the new theory has also been met with pronounced scepticism due, especially, to the deviation from standard physical theory. What is missing in order for Tsallis theory to win general recognition appears to be a convincing interpretation of the "mysterious"  $q$ -entropies. This is exactly where the research reported here claims to contribute.

Our approach involves a focus on concepts of *truth*, *belief* and *knowledge*, with knowledge conceived as the synthesis of extended *experience*. We appeal to game theoretical thinking involving two "players", *nature* and the *physicist*. The physicist seeks the truth, held by nature, but is restricted by his beliefs. After extensive observations, knowledge is gained. The physicist attempts to minimize *description cost*, whereas nature, following thoughts going back to Jaynes, has the opposite goal. *Entropy* is defined as the minimal achievable description cost.

Without going into technicalities, let us sketch the key ingredients of our approach. There are two, firstly considerations related to nature and outside the control of the physicist. This deals with the *world* the physicist operates in. Secondly, we shall work with *description* which, ideally, is under the control of the physicist. As to the first element, it rests on the assumption that there is an *interaction* which, given truth ( $x$ ) and belief ( $y$ ) determines knowledge ( $z$ ). If the interaction is given by  $z = x$ , we operate in the *classical world*, whereas the interaction  $z = y$  is taken to define a *black hole*. Interactions which are mixtures of these extremes are taken to define *Tsallis worlds*.

Then, concerning description, this rests on the assumption that every observation is connected with a *description cost*. This is defined in a probabilistic setting and is taken to depend on the probability of the *events* described. The *total description cost* takes all events (you may think of pure states) into account. The physicist can choose between various description strategies, characterized by a *descriptor*. In calculating the expected total description cost, the physicist has to base calculations on his belief and, of course, on knowledge of the world, he operates in. In order to choose an optimal descriptor, we rely on a basic variational principle which says that *description cost is the smallest when belief matches truth* ( $y = x$ ). This is the *perfect match principle* (PMP).

When you express the indicated principles in a formal mathematical way, you will find that the possible pairs of an *interactor*, characterizing the interaction, and the associated descriptor (determined via PMP) leaves you with a certain family parametrized by a parameter  $q \geq 0$ . The corresponding entropy functions are indeed

the Tsallis  $q$ -entropies. Except for a positive factor, we can write the Tsallis  $q$ -entropy of a probability distribution  $x = (x_i)$  as  $S_q(x) = \sum_i x_i \ln_q \frac{1}{x_i}$  with  $\ln_q$  the  $q$ -logarithm given by  $\ln_q(t) = \frac{1}{1-q}(t^{1-q} - 1)$  for  $q \neq 1$  and as the ordinary natural logarithm for  $q = 1$ .

The following statements will be considered critically:

- the interpretation given behind Tsallis entropy, building on interaction and description, is the most satisfactory one at this point in time;
- however, the new theory is not complete, especially the arguments leading to the various types of interaction are not entirely convincing and, furthermore, a clear connection to description via a process of *coding* as known from the Boltzmann-Gibbs-Shannon theory is lacking;
- *entropy by itself is incomplete*; in order to make sense, entropy must be complemented by other entities, such as description cost or *divergence*.

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## C.20 The monomer density profiles across the slit: Massive field theory approach

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The massive field theory approach in fixed space dimensions  $d = 3$  is extended to investigation of dilute solution of long-flexible polymer chains in a good solvent between two parallel impenetrable walls. Taking into account the well known correspondence between the field theoretical  $\phi^4$   $O(n)$ -vector model in the limit  $n \rightarrow 0$  and the behavior of long-flexible polymer chains in a good solvent allowed to calculate up to one-loop order the gyration radius components parallel  $R_{g\parallel}$  and perpendicular  $R_{g\perp}$  to the walls as well as the monomer density profiles for different regions  $L \gg R_g$  and  $L \ll R_g$ , where  $L$  is distance between the walls and  $R_g$  - the gyration radius of polymer chain in unrestricted region. Calculation of the monomer density profiles was performed for different cases of monomer-surface interaction: two repulsive walls, two inert walls and combination of one repulsive and one inert wall. The obtained results are in qualitative agreement with previous theoretical investigations and with

results of Monte Carlo simulations for the case of two repulsive walls.

## C.21 Cross-over of universality class in the Ising chain frustrated by long-range interactions

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We investigate a spin chain in which the ferromagnetic nearest-neighbor exchange interaction  $J$  competes with a long-range antiferromagnetic interaction of strength  $g$  decaying spatially as  $1/r^\alpha$ . For  $\alpha$  smaller than a certain threshold  $\hat{\alpha}$  (with  $\hat{\alpha}(J/g) > 2$ ), the long-range interaction is able to avoid the global phase separation – the uniformly magnetized state favored by the exchange interaction – even at  $T = 0$ . The ground state then consists of an ordered sequence of segments with equal length and alternating magnetization, resulting in a superlattice of magnetic domains [1]. A memory of this periodic spin profile is retained at finite  $T$  in the two-point correlation function, which oscillates as well but with a temperature-dependent period. Such an oscillation is then exponentially dumped over a spatial scale, the correlation length, which diverges asymptotically, roughly, as the inverse of  $T$ . This suggests that the long-range interaction drives the Ising chain to acquire a universality class consistent with an underlying continuous symmetry. The  $e^{\Delta/T}$ -temperature dependence of the correlation length and the uniform ferromagnetic ground state, characteristic of the  $g = 0$  discrete Ising symmetry, are recovered for  $\alpha > \hat{\alpha}$ . The relevance of our findings for the 2d dipolar frustrated Ising ferromagnet, whose ground state is again given by a mono-dimensional modulation of the order parameter [2], will be also discussed in relationship with experimental results on ultrathin Fe/Cu(001) films [3, 4, 5].

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## C.22 Evidence for an unconventional universality class from a two-dimensional dimerized quantum Heisenberg model

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A two-dimensional staggered dimerized quantum Heisenberg model is studied on the square lattice by means of (stochastic series expansion) quantum Monte Carlo simulations as a function of the coupling ratio  $\alpha = J'/J$ . The critical point of the order-disorder quantum phase transition in the staggered model is determined as  $\alpha_c = 2.5196(2)$  by finite-size scaling for up to approximately 10 000 quantum spins. By comparing the finite-size scaling of six dimerized models we show, contrary to the current belief, that the critical exponents of the staggered model are not in agreement with the three-dimensional classical Heisenberg universality class.

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## Abstracts of Posters

## P.1 Study of the conformational changes of hydrophobic-polar polymer chain near a hydrophobic chain

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Protein folding and binding are analogous processes, in which the protein searches for favourable intramolecular or intermolecular interactions on a funnelled energy landscape and the biological function of a protein is strictly related to its three-dimensional structure in the folded state [1, 2]. The theoretical treatment of this kind of works within the framework of statistical mechanics has been a longstanding problem that still gains a lot of interest [3, 4]. In this work, we focus on the interaction between two chains by using one of the effective off-lattice models of AB type [5] for polymers with  $N$  monomers. We add a second chain as a fixed chain in the simulation. The second chain was set up as a homopolymer and is attractive to other polymer chain sequences. For calculating the new energy of the hydrophobic-polar chain, Lennard-Jones type potentials are assumed as the interaction term between the fixed chain and the AB chain. We put the other chain in a specific distance from fixed chain and we determine the minimum energies and specific heats for this new systems.

Acknowledgements: H. Alaboz and H. Arkin acknowledges support by The Scientific and Technological Research Council of Turkey under the project number 104T150 and H. Arkin acknowledges The Turkish Academy of Sciences under the programme to Reward Successful Young Scientists.

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## P.2 Free energy inherent structures in spin glass models

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One important feature of the glass phase of spin glasses is its rugged energy landscape. Whereas at zero temperature the (possibly degenerate) ground state dominates, local energy minima with higher minimum energy and the entropy of the corresponding valleys become important at higher temperatures. Especially the congruational entropy (the complexity) of the spin glass at different temperatures is of interest. These quantities can be obtained from Monte Carlo simulations using the free energy inherent structure (FEIS) approach introduced in Ref. [1]. This method is applied to the Sherrington-Kirkpatrick (SK) model and the Edwards-Anderson Ising (EAI) model, both with a bimodal distribution for the couplings. The application of the multi-canonical algorithm allows to simulate bigger system sizes for the SK model than before, while the EAI model has not been studied by this method before.

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## P.3 Formation of a plateau in the twist order parameter of the bond alternating antiferromagnetic $S = 1/2$ Heisenberg spin chain

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The twist order parameter was introduced in [1] to signal a quantum phase transition between different valence bond configurations in various 1D quantum spin systems. We present quantum Monte Carlo simulations combined with quantum reweighting methods. At non-zero temperature we find the formation of a plateau in the twist order parameter around the (zero temperature) quantum critical point. We investigate the possibility that this plateau is related to the quantum critical region that

fans out from the quantum critical point.

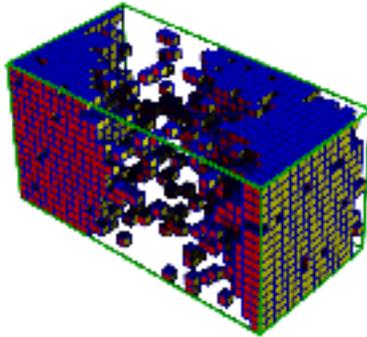
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## **P.4 Anisotropy of the interface tension of the three-dimensional Ising model**

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We determine the interface tension for the 100, 110 and 111 interface of the simple cubic Ising model with nearest-neighbour interaction using novel simulation methods. To overcome the droplet/strip transition and the droplet nucleation barrier we use a newly developed combination of the multimagnetic algorithm with the parallel tempering method. We investigate a large range of inverse temperatures to study the anisotropy of the interface tension in detail.



Plot of a typical configuration with two 110 interfaces.

## P.5 Critical scaling in the fundamental theory of fluids

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The conventional statistical theory of fluids based on the integral equations for correlation functions allowed successful prediction of many thermodynamic properties of real liquids. Up to the last time, however, with the help of this theory one failed to obtain a plausible, consistent with experiment and calculations by the lattice gas model, description of the singularities of thermodynamic quantities near the gas-liquid critical point. In the authors recent paper [1] it was demonstrated, for the first time, that the fundamental equations of the theory of fluids admit solutions from which the critical singularities of the Ising type follow. Three critical exponents ( $\eta = 1/5$ ,  $\nu = 5/8$ ,  $\gamma = 9/8$ ; cf. with the corresponding classical values: 0, 1/2, 1) were calculated, independently. These exponents together with those recovered using the well-known relations between the exponents are in good agreement either with the experimental values for real fluids or with the numerical calculations for the 3D Ising model and by the  $\epsilon$ -expansion method. In the present communication, there outlined the ways of independent calculation of main critical exponents starting from the fundamental theory of fluids. It means that the results of this theory agree with those following from the Kadanoff-Wilson-Fisher scaling approach.

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## P.6 Stochastic tumor growth with immunization

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Tumor diseases increasingly gain in importance during the past decades. Much effort has been spent on revealing the mechanisms of tumor evolution. Researchers found out that the immune system can influence tumor development in a significant manner.

Based on this findings, we analyze tumor growth and the interaction of cancer cells with the immune system. A deterministic component as well as a random nature is attributed to the tumor-immune interaction.

More specifically, we study a stochastic model for tumor cell growth with both, a multiplicative and an additive noise term as well as cross-correlations in between. The noise includes a finite correlation time. Whereas the death rate within the logistic model is altered by a deterministic term characterizing immunization, the birth rate is assumed to be stochastically changed due to internal growth processes leading to a multiplicative internal noise. Additionally the system is subjected to an external additive noise which mimics the influence of the environment of the tumor including the stochastic elements of the immune response. The stationary probability distribution is derived to analyze the influence of finite correlation time, the immunization rate and the strength of the cross-correlation on the different steady states. Furthermore, the mean-first passage time is calculated in order to find out under which conditions the tumor can suffer extinction under the effect of correlated noise and the degree of immunization.

## **P.7 Adsorption and recognition of multiblock co-polymers on chemically heterogeneous, patterned surfaces**

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The results of Monte Carlo simulations on a system of multiblock copolymers on a checkered surface are presented here. The statistical, thermodynamical and conformational properties are studied. We have found that a two-stage pattern recognition happens with multiblock copolymer forming multiple pinning sites on the boundary between the different surface sites. The conformational properties show interesting effects with the perpendicular component showing strong deviations from the standard behaviour.

## P.8 Finite size effect in persistence in random walk

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The phenomenon of persistence has attracted a lot of attention in recent times. Persistence is the characteristic of stochastic process and as the name suggests it conveys the meaning of “Survival” To quantify this survival we define the persistence probability  $p(t)$  which is simply the probability that the local field has not changed sign upto time  $t$ . Of all the stochastic process the simplest of them, the random walk model exhibits this persistence phenomenon and the persistence probability decays as  $p(t) \sim t^{-\theta}$  with  $\theta = 1/2$ . The present study we will be presenting here is motivated by the experimental work of Lukić et al. where they have experimentally observed non-diffusive behavior in Brownian motion using optical traps. Since in experimental situations the size of the boundaries come into play, we have therefore investigated the effect of finite size in the persistence probability and how the probability scales with the finite size parameter. This has been done in two ways, first the random walker was confined in in box of size  $2L$  and in the second case the walker is trapped in a harmonic potential. In both cases analytical and numerical calculation show that the scaling function is exponentially decaying.

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## **P.9 Reversibility and its influence in quantum communication**

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The off resonance effect and its influence on the reversibility between two quantum subsystems in interaction (single mode cavity field and a three-level atom in cascade configuration) are studied. A new model of quantum communication and the influence of the reversibility on its realization is studied. The partial restoration condition is found at which these radiators can restore their diagonal moments, while the non-diagonal ones remain correlated after the interaction process.

## **P.10 Density scaling of the dynamics and pressure-energy correlations in hard and soft matter**

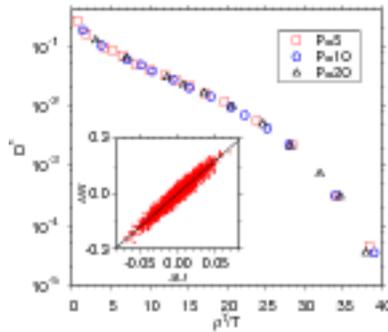
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Density scaling of dynamic properties is experimentally observed in a wide class of highly viscous liquids, including polymeric and molecular glass-formers. From the theoretical point of view, this feature is well-studied for fluids where particles interact via inverse power-law (IPL) potentials. The latter systems also display exact correlations between pressure and energy fluctuations. During the last year, the link between approximate density scaling of the dynamics, strong pressure-energy correlations and IPL approximations of the interaction potential has been actively investigated on the basis of computer simulations [1, 2, 3, 4]. In this contribution, I will review these findings for simple models of glass-forming liquids based on  $m$ -6 Lennard-Jones potentials ( $8 \leq m \leq 36$ ), i.e., including an attractive component in the potential. I will show that both thermodynamic scaling and pressure-energy correlations reflect the validity of IPL approximations of the interaction potential in the relevant range of interatomic separations. Finally, I will address the question if scaling laws can be extended to models in which particles interact with an ultra-soft, bounded potential (generalized exponential model), as they are, for instance,

encountered as effective interactions in polymers, or other colloidal dispersions. For such “soft” systems, density scaling is predicted by mean field approaches, but its nature turns out to be different than in “hard”, atomic matter.

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Main figure: density scaling of reduced diffusion coefficients  $D^*$  for a binary Lennard-Jones mixture with repulsive exponent  $m = 8$ .  $D^* = (\rho^{1/3}T^{-1/2})D$  is shown as a function of  $\rho^\gamma/T$ , where  $\rho$  is the density,  $T$  is the temperature, and  $\gamma = 3.5 \pm 0.1$  is an effective scaling exponent. The latter has been determined so as to maximize the overlap between data sets corresponding to different pressures  $P$ . Inset: correlation between instantaneous fluctuations of the virial  $W$  and of the potential energy  $U$  for the same system at a representative state point ( $P = 10$ ,  $T = 0.62$ ). The slope obtained by linear regression is  $\Gamma = 3.6$ , in good agreement with the scaling exponent  $\gamma$ .

## P.11 Ground state of anisotropic antiferromagnets with single ion and cubic anisotropy

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Anisotropic antiferromagnets in an external magnetic field show a rich variety of different phases meeting in phase transition lines and multicritical points. We study the dependence of the ground states of these systems in the three dimensional space on physical parameters as exchange, single ion and cubic anisotropy (see [1, 2]).

One identifies four different ground states: the paramagnetic, the antiferromagnetic, the spin flop and the biconical ground state. In the case of absence of a cubic anisotropy the transition lines separating the different ground states can be calculated analytically, otherwise they have to be calculated numerically. We also considered the behavior of the staggered magnetization which characterizes the different ground states. From its behavior the order of the transition from one state to the other is determined.

The results obtained may be relevant for other systems since the antiferromagnetic model can be mapped to a lattice model where the biconical phase is interpreted as supersolid phase [3]. Recent renormalization group calculations show that such a phase would indicate the existence of a tetracritical point [4].

Acknowledgement: We thank W. Selke for valuable discussions. This work was supported by the Fonds zur Förderung der wissenschaftlichen Forschung under Project No. P19583-N20.

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## P.12 Application of the confined quantum field theory in statistical physics

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Confined Quantum Field Theory solves some fundamental problems in physics like the conflict between the theory of the relativity and the quantum field theory. Concerning statistical physics is its simple description of superconductivity and superfluidity, which is a transition from disorder to order movement of the conducting electrons. CQFT establishes a relation between the metric of the quantum domain and the energy density, therefore the energy of the electron dictates the radius of confinement. The elements of the superconductivity are electrons with radius of confinements coincide with some number of periods of the bulk. Ordered movement of the conducting electrons preserves the periodicity. We show that in fact the Boltzmann equation can be used to describe this transition.

## P.13 Shapes of two dimensional star polymers

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We explore the shapes of excluded volume, two dimensional star polymers by both renormalization group methods and Monte Carlo computer simulation of a tangent hard disk model. The mean-square radius of gyration, the  $g$ -ratio and the asphericity of linear and star polymers are examined. The standard expansion for the  $g$ -ratio is modified to use the known exact value of the radius of gyration exponent  $\nu = 3/4$  rather than only the first order  $\epsilon$ -expansion value. Good agreement is obtained with the current Monte Carlo Pivot algorithm results and previous simulations of other polymer models. Our approach also improves the predictions of the  $g$ -ratio in three dimensions significantly enhancing the accuracy of the renormalization group results

for calculating shape properties.

## **P.14 DNA bubble dynamics as a quantum Coulomb problem**

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We study the dynamics of denaturation bubbles in double-stranded DNA on the basis of the Poland-Scheraga model. We demonstrate that the associated Fokker-Planck equation is equivalent to a Coulomb problem. Below the melting temperature the bubble lifetime is associated with the continuum of scattering states of the repulsive Coulomb potential, at the melting temperature the Coulomb potential vanishes and the underlying first exit dynamics exhibits a long time power law tail, above the melting temperature, corresponding to an attractive Coulomb potential, the long time dynamics is controlled by the lowest bound state.

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## **P.15 Bethe approximation for a DNA-like self-avoiding walk model with variable solvent quality**

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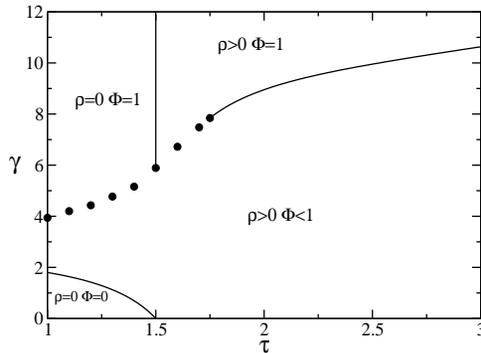
The phase diagram and critical behaviour of a simple toy model for DNA zipping/unzipping is examined in the framework of the Bethe approximation. The effects of solvent quality are included, and found to lead to a variety of different thermodynamic behaviours.

The thermodynamic behaviour may be investigated by introducing the grand-canonical partition function,  $\mathcal{Z}$ , from which many of the relevant thermodynamic quantities may be calculated. The grand-canonical partition function is given by:

$$\mathcal{Z} = \sum_{\text{walks}} K^N \tau^{N_I} \gamma^{N_2}$$

where  $N_I$  is the number of solvent-mediated interactions,  $N_2$  is the number of doubly visited bonds, and  $\tau$  and  $\gamma$  are the associated Boltzmann weights. The fugacity, which controls the average length of the walk, is denoted by  $K$ .

A variety of different multicritical points are observed, both in the high- $K$  dense phase and on the  $K_\infty$  plane, where the walk's length just diverges.



Phase diagram in the  $K_\infty(\tau, \gamma)$  plane. The density is denoted by  $\rho$ , and  $\Phi$  denotes the proportion of paired bonds.

## P.16 Phase transition in doped crystals

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We analyze results of the data on neutron diffraction research in structures of paramagnetic and magnetic phases in doped crystals undergoing phase transition and present dependence of critical indices of the magnetic phase transitions of these systems as function of doped atoms concentration. Besides, research of structures of paramagnetic and magnetic phases in the same compounds show that with changes

of the doped atoms concentration, the symmetry space group of high-symmetry and low-symmetry phases remains unchanged. We consider a case when distribution of defects in structure induced small-world property [1] and show that due to this the distribution function of the order parameter defined by Fokker-Plank equation has form of the Tsallis distribution  $p(k)$ . The equation of motion for the order parameter is defined from the extreme principle of the free energy functional

$$\int_0^t dt' p_0(t-t') \frac{\partial \eta(x, t')}{\partial t'} + \int_{-\infty}^{+\infty} dy p_1(x-y) \frac{\partial \eta(y, t)}{\partial y} + \frac{\partial F(\eta(x, t))}{\partial \eta(x, t)} = 0,$$

where  $F(\eta(x, t))$  depends on invariants of an irreducible representation of space group of a paramagnetic phase which defines transformational properties of the order parameter  $\eta(x, t)$ . We derive the fractional equation of motion for the order parameter and obtain the nonlinear dispersion law. Then we present a renormalization group analysis of magnetic phase transitions in doped crystals. We have solved the corresponding equation of the renormalization group and defined critical indices of the system near phase transitions. We have determined the dependence of critical indices on the nonextensivity parameter of the system. We obtain explicit dependence of nonextensivity parameter from fractal dimension of system. Using  $\varepsilon$ -expansion for solution of the equation of motion we show, that with a change a concentration of doped atoms is possible a phase transition in an incommensurate phase of doped crystals.

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## P.17 A liquid state approach to biopolymers

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Solutions of stiff biopolymers have unique properties which rely on the fact that the filaments are neither completely rigid nor completely flexible. A successful description of their equilibrium properties is based on the concept that hard-core interactions with the surrounding solution confine each polymer to an effective tube-like cage. The tube radius plays a central role for the phenomenology of stiff polymer solutions. Its scaling behavior with concentration as well as exact prefactors have

been derived using mean-field theory and simulation. Generalizing Onsager's ansatz for hard cylinders, we propose a liquid-state theory for stiff polymers which allows one to derive the fluctuations of the tube radius itself. The results compare favorably to dynamical measurements on F-actin networks, obtained using confocal laser scanning microscopy.

## **P.18 Historical introduction of the effective interactions approach in the statistical mechanics of multicomponent liquid systems: Einstein's brownian paper of 1905**

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In his paper about the brownian motion published in 1905 [1], Einstein presented a derivation of the Van't Hoff law for the osmotic pressure of the suspended (solute) particles. The derivation was based in his own version of the statistical mechanics in the canonical ensemble. This result has been scarcely cited and discussed but constitutes the first use (at least in an implicit way) of the so called effective interactions approach in liquid physics [2]. In this work, the method used by Einstein is analyzed, the implicit assumptions discussed and the adequate formulation of the thermodynamics presented. Posterior extensions and/or versions of this approach by R. H. Fowler (1929), E. A. Guggenheim (1932), L. Onsager (1933), G. S. Rushbrooke (1940), I. M. Lifshitz & G. I. Stepanova (1957), L. D. Landau & E. M. Lifshitz (1958) and others will be briefly mentioned leading a formulation of the effective interactions approach in the canonical ensemble. Finally, the thermodynamics that can be derived from the corresponding effective canonical partition function is presented jointly with the comparison with the experiment.

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## **P.19 Theoretical investigation of a DDW-DSC hamiltonian for $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$**

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A momentum space mean field DDW-DSC Hamiltonian for  $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$  is investigated self-consistently for a reasonably wide temperature and doping range. A relation between thermodynamic potential of the system and certain spectral weight functions is established. The relation is found to be useful for deriving finite temperature thermodynamics of the system. For the Fermi surface(FS) reconstruction exercise in the normal state, the bi-layer splitting is included by the parametrization in terms of a momentum conserving tunneling matrix element. This splits the electron pockets whereas the lower branch of the excitation spectrum remains unaffected. In the mean field approximation framework, the spectral function at the anti-nodal points of FS is analyzed in the absence and the presence of magnetic field. The latter shows two prominent frequencies of the Shubnikov de Haas oscillation. The oscillation amplitude too is found to be mildly magnetic field dependent broadly confirming to the Lifshitz-Kosevich model for the oscillation in magnetization, is also discussed.

## **P.20 Analytical and computational study of the heterogeneity in complex systems**

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Complex systems typically have the following characteristics. First, they consist of a large number of agents interacting with each other in many different ways. Secondly, interest focuses on collective properties of the system as whole, which may result in emergent structures of great complexity at larger scales or after long times. Thirdly, random or stochastic effects are important: both determinism and chance are needed to describe the reality. Because of the real limitations of the use of analytical methods to study such problems, it often necessary to resort to numerical methods, and the advent of computer simulations has led to an increase of scientific activity in this area that has emerged nowadays as a major subject of interdisciplinary research [1].

The purpose of this study is to consider the model proposed in [2] in the case of a system formed by  $N$  agents with  $P(N)$  possible partitions into six clusters over three different states, and to show that even for a small number of agents  $N = 100$ , with  $P(N) = 96,560,646$  possible partitions, obtained files becomes of order about 100 Mb and there is a huge problem of processing such a files due to restriction of the computer memory. Due to this restriction of the computer memory, it is not possible to process such a program on ordinary computers, so the need of parallel programming is obvious even in a case of a simple model concerning the behaviour of complex systems.

The model describes the interactions in a complex heterogeneous system of agents. In particular, there are  $N$  entities which can be in 3 different states, and can perform 3 actions. One can identify 6 different combinations denoted with probabilities  $p_1 \dots p_6$ . That is, drawing randomly one agent, it will be of type  $i$  with probability  $p_i$ . Let  $N = 1, 2, \dots, \infty$  be the total number of entities in the model, and  $n_1, n_2, n_3, n_4, n_5, n_6$  is their partition into  $m = 6$  subsets. Each subset can be called *cluster*, and the process itself - *clustering*. The size of each cluster can vary from 0 to  $N$ ,  $n = \overline{0, N}$ ,  $i = \overline{1, 6}$  and  $\sum_{i=1}^6 n_i = N$ . The number of possible partitions  $P$  is a function of  $N$ , and the solution is  $P(N) = \frac{1}{5!} \prod_{i=1}^5 (N + i)$  [2]. Note that there are  $N(p_1 + p_2)$  similar entities in the ensemble. So the number of partitions  $P$  depends on the number of agents and increases as a product. In general,  $P(m, N) = \frac{1}{(m-1)!} \prod_{i=1}^{m-1} (N + i)$ .

Some set of probabilities  $p_1 \dots p_6$  have been simulated during calculations. Choose of the step for creating all combinations of probabilities gives the total number of agents in the system, for example, if the step is 0.001, then the total number of agents is 100 and the number of partitions  $P$  will accordingly be 96,560,646. The problem then was to process this set of data and to average it over many different values.

Finally, we would like to point out that the model considered above is a general one and allows simulations for any size of the system, but due to restriction of computer memory it works only for the small number of agents. Using this model it is possible to study agent-based interactions in complex heterogeneous systems with different applications, so the need of parallel programming to perform such computations is obviously.

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## P.21 Diffuse damage and single crack growth in sub-critical fracture

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Disordered materials subject to sub-critical external loads present a time dependent macroscopic response and typically fail after a finite time. Such time dependent fracture evidently plays a crucial role in a large variety of physical, biological, and geological systems, such as the rupture of adhesion clusters of cells in biomaterials, the creep and fatigue fracture of materials and the emergence of earthquake sequences [1].

We present a detailed theoretical study of the fracture of disordered materials subject to a constant external load. We worked out a fiber bundle model, which provides a direct connection between the microscopic fracture mechanisms and the macroscopic time evolution of the system. In the model, fibers fail either due to immediate breaking or undergo a damage accumulating ageing process [2, 3]. After a failure event, the load of the broken fibers is redistributed locally over their intact nearest neighbors. Since load redistribution and immediate breaking occur on a much shorter time scale than damage accumulation, the entire fracture process can be viewed on the microlevel as a sequence of bursts of immediate breakings triggered by a series of damage events happening during waiting times, *i.e.*, the time intervals between the bursts. Due to the localized interaction of fibers, the bursts and damage sequences are spatially correlated giving rise to growing clusters of broken fibers [2, 3].

We show that the interplay of threshold disorder and of the inhomogeneous stress field gives rise to a rich dynamics with intriguing novel aspects. When the disorder is strong a high amount of damage occurs randomly scattered over the system, however, for weak disorder a single growing crack is formed which proceeds in a large number of localized bursts. Along the boundary of the two phases in the phase diagram, the size distribution of micro-cracks in the critical state has a power law behavior with an exponent close to the cluster size exponent of percolation. In the regime of single crack propagation, the size of bursts and the waiting times between consecutive bursts have universal power law distributions. Creep experiments were carried out on paper using the acoustic emission technique. The energy of acoustic signals and the inter occurrence times were found to follow power law distributions with exponents in a reasonable agreement with the theoretical predictions.

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## P.22 Non-equilibrium kinetics and ageing in non-glauberian Ising models

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The exactly solvable one-dimensional kinetic Ising model with Glauber dynamics has served since a long time as an useful pivot for studies in non-equilibrium cooperative behaviour. Recently, we have shown that for the case of the kinetic Ising model with Kimball-Deker-Haake dynamics, it is possible to derive exact results for several two-time correlation and response functions [1]. In particular, the non-equilibrium exponents, which describe the ageing behaviour, can be extracted. From these, it can be seen that the two types of dynamics are in different universality classes.

We shall also describe attempts to generalise beyond these two known dynamics [2].

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## P.23 Entanglement entropy of quantum spin chains

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We consider two prototypical quantum models, the spin-1/2 XY chain and the quantum Ising chain and study their entanglement entropy,  $S(\ell, L)$ , of blocks of  $\ell$  spins in homogeneous or inhomogeneous systems of length  $L$ .

- i) We show an exact relationship between the entropies and translate existing exact results [1].
- ii) For the homogeneous quantum Ising chain with  $\ell = L/2$  we define a finite-size pseudo-critical point through the position of the maximum of the entropy and study its scaling properties [2].
- iii) We consider a gradient in the systems through a linear variation of the couplings and study the evaluation of the entropy in time after quenching to a homogeneous critical system [3].

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## P.24 Superdiffusion in a class of networks with marginal long-range connections

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A class of cubic networks composed of a regular one-dimensional lattice and a set of long-range links is introduced. Networks parametrized by a positive integer  $k$  are constructed by starting from a one-dimensional lattice and iteratively connecting each site of degree 2 with a  $k$ th neighboring site of degree 2. Specifying the way pairs of sites to be connected are selected, various random and regular networks are defined, all of which have a power-law edge-length distribution of the form  $P_{>}(l) \sim l^{-s}$  with the marginal exponent  $s = 1$ . In all these networks, lengths of shortest paths grow as a power of the distance and random walk is super-diffusive. Applying a renormalization group method, the corresponding shortest-path dimensions and random-walk dimensions are calculated exactly for  $k = 1$  networks and for  $k = 2$  regular networks; in other cases, they are estimated by numerical methods. Although,  $s = 1$  holds for all representatives of this class, the above quantities are found to depend on the details of the structure of networks controlled by  $k$  and other parameters.

## P.25 Modeling bursting processes by the nonlinear stochastic differential equations

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Many complex systems exhibit quiet periods separated by bursts, i.e., events of rapid evolution. Such systems often produce noise with the power-law characteristics, which can be modeled in terms of avalanches [1, 2, 3]. Here we will present modeling by the nonlinear stochastic differential equations [4] of scaled processes exhibiting bursts characterized power-law distributions of burst size, burst duration and the inter-burst time, as in a case of avalanches in self-organized critical (SOC) models and the extreme event return times in long-term memory processes.

The generated signal itself exhibit the power-law distributions of the signal intensity,  $1/f^\beta$  noise, power-law autocorrelations and second order structural (height-height correlation) functions. The proposed model reproduces  $1/f$  noise and the processes in SOC and crackling systems and it is also related to the clustering Poisson process,  $1/f$  noise in nanochannels, single-channel and ion channel currents, etc and may be used for simulation of long-range scaled processes exhibiting  $1/f$  noise, power-law distributions and self-organization.

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## P.26 Bosons in a box: More precise expression of the excited states population

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We consider a system of free bosons in a box. We calculate the population of the excited states using the exact non vanishing energy of the ground state energy, in place of the vanishing value used previously in the literature. We obtain a more precise expression for this population. This gives us a more accurate value for the critical temperature of the Bose Einstein condensation.

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## P.27 Spreading of innovations on complex networks of agents

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Technological evolution of socio-economic systems has two major components [1]: (i) *Innovation* New products, ideas, paradigms emerge as a result of innovations which are then tested by the market. (ii) *Spreading* Successful technologies spread over the system resulting in an overall technological progress. The spreading of technological advancements is typically preceded by the spreading of information about the existence and advantages of the newly developed technology. This process is initiated by the advertising activities of the producers and providers of the new product resulting in a vertical information flow into the system. As to the next, information spreads laterally through the communication of individuals.

We study the spreading of information in socio-economic systems using an agent-based model. The system is modelled as a collection of agents whose social contacts have a complex network topology. The behavior of agents is captured by two param-

eters which characterize the response of agents to the external driving emerging due to advertising activities, and to the word-of-mouth communication with their social partners. Analytic calculations and computer simulations revealed a rich spectrum of novel behaviors varying the parameters of the model and the underlying network topology of agents' social contacts. Agents with a high sensitivity to external advertising serve as nucleation centers from which clusters of informed agents grow. The gradual nucleation and grows of clusters lead to merging which in turn results in the appearance of a macroscopic cluster connecting nearly all informed agents. We show numerically that the transition from the phase of disconnected growing clusters to the phase of a macroscopic cluster of informed agents is analogous to second order phase transitions. Simulations were carried out on a Watts-Strogats network varying the rewiring probability starting from a square lattice. At the critical time  $t_c$  of the phase transition the size distribution of clusters proved to be a power law with a topology dependent exponent  $\tau$ : on a square lattice the exponent is  $\tau = 1.75$ , however, increasing the rewiring probability a crossover occurs to a higher exponent  $\tau = 2.5$ . The critical exponent characterizing the divergence of the average cluster size at  $t_c$  depends also on the topology.

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## **P.28 Griffiths-McCoy singularities in random quantum spin chains: Exact results**

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Quenched disorder has a profound effect on the low-energy, low-temperature and long wavelength properties of quantum systems. The interplay between quantum fluctuations, correlations and disorder fluctuations generally results in strong singularities of the thermodynamical quantities. This type of effect takes place even outside the quantum critical region, in the so called Griffiths-phase. We used a direct and simple method to calculate exact values of the Griffiths-McCoy singularities in a class of random quantum spin chains, including the tight-binding chain, the anti-

ferromagnetic  $XX$ -chain as well as the transverse-field Ising chain. Our results are obtained from the density of states of the low-energy excitations, which is calculated exactly by the Dyson-Schmidt method. In large finite systems the low-energy excitations are shown to follow the statistics of extremes and their distribution is given by the Fréchet form. Relation between the Dyson-Schmidt technique and the strong disorder renormalization group method is also discussed.

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## P.29 Inelastic relaxation in sticky biopolymer networks

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Living cells exhibit a highly characteristic reproducible linear and nonlinear rheological response that displays viscoelastic stiffening, inelastic creep and kinematic hardening [1]. Recent experimental observations [2] trying to isolate the inelastic creep of living cells from the better understood viscoelastic response demonstrate that preconditioning by transient stretching causes softening as opposed to the known viscoelastic stiffening. We propose a simple unified theoretical explanation of these somewhat puzzling experimental observations based on the glassy wormlike chain model [3].

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## **P.30 Coupling of orthogonal diffusion modes in two-dimensional inhomogeneous systems**

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Collective diffusion coefficient in a two-dimensional lattice gas on a nonhomogeneous substrate is investigated using variational approach. In our model particles reside and jump randomly between adsorption sites modeled as potential wells with different depths. Site blocking is the only allowed particle-particle interaction mechanism. It is shown that the value of the diffusion coefficient in one lattice direction depends nontrivially on the rate and the character of the particle jumps in other directions. The collective diffusion coefficient increases, eventually approaching values predicted within the mean-field approximation when the jump rate increases in the direction perpendicular to that in which the diffusion coefficient is measured. Analytical predictions of our model are supported by the Monte Carlo simulation performed for selected systems.

## **P.31 Zipf's law and Potts model**

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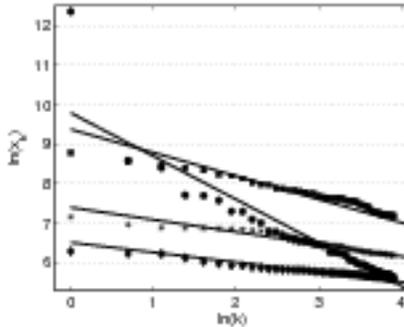
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The domains statistics has been an attractive field of research in the past few years [1, 2, 3]. Zipf's power law and its connection with the inhomogeneity of the system is investigated. We describe Zipf's power law in the Potts model near the temperature-induced phase transition and beyond it. It appears that Zipf's index is approximately equal 1 in the critical region.

We found that the statistical distribution of the domain masses in the critical point is described by the Pareto power law with long tail, while beyond the critical point the power law is suppressed.

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The log-log distribution of domain masses  $x_k$  versus the rank index  $k$  for the 3-state Potts model.

## P.32 Exact solution of the extended Hubbard model in the atomic limit on the Bethe lattice

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We study the phase diagram at finite temperature of a system of Fermi particles living on the sites of a Bethe lattice with coordination number  $z$  and interacting through onsite  $U$  and nearest-neighbor  $V$  interactions. This is a physical realization of the extended Hubbard model in the atomic limit [1]. By using the equations of motion method, we provide a comprehensive and systematic exact analysis of the model by considering all the relevant response and correlation functions as well as thermodynamic quantities for attractive and repulsive intersite and on-site potentials [2, 3]. We determine the complete phase diagrams in the  $(U/V, n/V, T/V)$  space and we find, for both negative and positive  $V$ , a critical temperature separating a homogeneous translational invariant phase from a state with phase separation and a charge ordered state, respectively. Relevant thermodynamic quantities - such as

specific heat, susceptibility, entropy – are also investigated as functions of the temperature, on-site potential and particle density.

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## **P.33 Many-particle approach to multiferroic bulk systems**

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Multiferroic bulk systems are studied in a many-particle approach. Starting from a microscopical description the temperature dependent excitations and the associated damping of ferroelectric and magnetic modes are calculated. Polarization, magnetization and dielectric function, as the macroscopic quantities are determined by the microscopic behavior. An anomaly in the ferroelectric quantities close to the magnetic phase transition is observed. The analysis of the ferroelectric subsystem is based on a two-state quantum model, the Ising model in a transverse field. The magnetic moments interact via the Heisenberg model. The corresponding multiferroic coupling term differs for hexagonal and orthorhombic materials. A Green's function technique in reciprocal space provides the static and dynamic properties. The theoretical result are compared with experimental data.

## P.34 Statistical description of classical systems by considering finite instrumental resolution scales

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By considering classical systems whose parameters are measured with finite instrumental resolution scales we have to assume that particles coordinates on these scales are indistinguishable [1, 2, 3]. As result such particles' systems are characterized by joint probability that  $N$  particles occupy a probing volume. Therefore system's parameters are defined on the base of  $N$ -particle probability functions  $f_N$  as against classical one-particle definitions. In addition the reduced probability functions  $f_N$  are calculated under assumption about indistinguishability of particles coordinates within probing volumes what also is different from the classical theory. The suggested approach results in description of particles' systems in terms of fluctuations of system's parameters.

The presented conception avoids Gibbs paradox and provides within its own formalism the transition from classical statistical integral to quantum statistical sum by respective decrease of instrumental resolution scales.

This description applied to neutral gases produces under some assumptions classical one-particle definitions of mean parameters. In contrast, for systems with long-range interactions (e.g. Coulomb systems) such definitions remain to be multiparticle (what depends on number of particles on interaction scales).

The presented multiparticle statistical approach is tested by some classical problems and illustrated by the problem of solar plasma expansion.

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## P.35 Coulomb gap revisited: A renormalization-like approach

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One of the most prominent features of the Coulomb glass is the soft gap in the single-particle density of states [1]. Previous numerical studies of the gap yielded densities considerable deviating from the analytical result [2, 3]. The aim of the present work is to contribute to the clarification of these deviations.

Because of the long-range interaction, the energy region which could be considered in previous simulations was restricted by severe difficulties arising from finite-size effects. To overcome this problem, we use a renormalization like procedure. It is not based on composing a large sample out of pre-relaxed small pieces but on introducing a cutoff length of the interaction which increases step by step during relaxation. The arising small error of the single-particle energies is considered to be a random correction to the random on-site field. In this way, simulations of samples of up to  $2 \cdot 10^9$  sites are performed.

For one- to three-dimensional samples, we study the influence of the disorder strength. The consideration of the extremely large samples opens new insight: There is a tendency to universal behavior in all three cases as predicted analytically. Asymptotic power laws with the predicted exponents seem to hold in the two- and three-dimensional cases, where the prefactors are by factors 2 and 3 smaller than predicted. However, this behavior is observed only in the region of very low energies.

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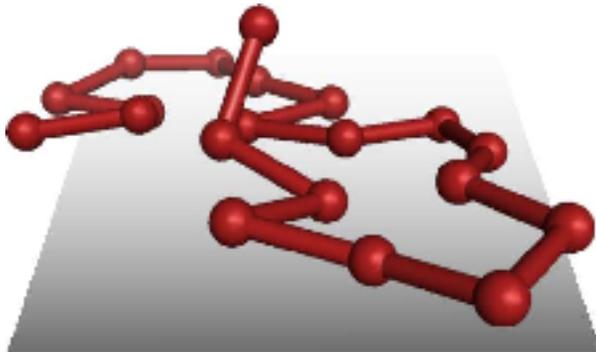
## P.36 Conformational mechanics of polymer adsorption transitions at attractive substrates

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Conformational phases of a semiflexible off-lattice homopolymer model near an attractive substrate are investigated by means of multicanonical computer simulations. In our polymer-substrate model, nonbonded pairs of monomers as well as monomers and the substrate interact via attractive van der Waals forces. We analyze thermal fluctuations of energetic and structural quantities and adequate docking parameters as a function of the temperature. Introducing a solvent parameter that is related to the strength of the surface attraction, we construct and discuss the solubility-temperature phase diagram. Apart from the main phases of adsorbed and desorbed conformations, several other phase transitions such as the freezing transition between energy-dominated crystalline low-temperature structures and globular entropy-dominated structures are identified.

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A typical conformation of an adsorbed 20mer.

## P.37 Rapidly switched random links enhance spatiotemporal regularity

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We investigate the spatiotemporal properties of a lattice of chaotic maps whose coupling connections are rewired to random sites with probability  $p$ . Keeping  $p$  constant, we change the random links at different frequencies, in order to discern the effect (if any) of the *time dependence of the links*. We observe two different regimes in this network: (i) when the network is rewired slowly, namely when the random connections are quite static, the dynamics of the network is spatiotemporally chaotic and (ii) when these random links are switched around fast, namely the network is rewired frequently, one obtains a spatiotemporal fixed point over a large range of coupling strengths. We provide evidence of a sharp transition from a globally attracting spatiotemporal fixed point to spatiotemporal chaos as the rewiring frequency is decreased. Thus, in addition to geometrical properties such as the fraction of random links in the network, dynamical information on the time dependence of these links is crucial in determining the spatiotemporal properties of complex dynamical networks.

## P.38 Monte Carlo generation of equilibrated graphs

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We propose a C++ library for generating and handling random graphs [1] with given statistical weights [2]. The modular and extendable set of functions allows the user to easily create a program that generates complex networks with prescribed node-degree distribution, node-node correlations and assumed global structure (trees, simple graphs or degenerated graphs), with no a-priori limitation on the size of graph. The library also contains functions to perform statistical estimations on graphs or

to export the graphs for further external processing or visualization [3].

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- [2] L. Bogacz, Z. Burda, and B. Waclaw, Physica A **366** (2006) 587.
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## **P.39 Patterns of chains in thick polymer condensates**

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We use a pattern recognition program in order to study conformational building blocks in the ground states of thick homopolymers with small length. The theory has two parameters, the polymers thickness and a radius  $r_0$ , denoting the minimum position of the Lennard Jones potential function. We present a study at values  $r_0 = 1.0$  and  $r_0 = 1.6$  and observe regions of thickness values with ground states, that either are simple cubes and helices, or planar sheets. The poster complements recent findings as published in [1] but also presents the technical details of pattern recognition along the ideas of [2] for the case of polymers.

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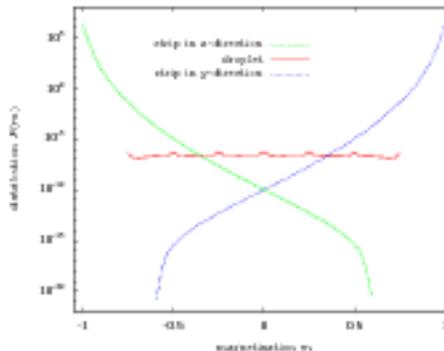
## P.40 A nearly local observable for a global quantity

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I will present recent results on the simulation of the two-dimensional  $L \times L$  Ising model at temperatures below the critical temperature  $T_c$ . Using a multimagnetical algorithm it is possible to obtain weights  $W(M)$  for all values of the magnetisation  $M$  that are inverse proportional to the distribution  $P(M)$ . During a simulation with these weights, the different values of  $M$  are visited in a random-walk like manner. Unexpectedly, this behaviour changes for larger system sizes and lower temperatures and block like structures show up in the time series of the magnetisation. An explanation for this phenomenon was given by [1] who realized that, as a consequence of the periodic boundary conditions of the simulation, the system must perform a transition from droplet to strip configurations (and vice versa) in order to visit all magnetisations. To overcome the barrier that is associated with the transition, we present a new Ansatz, where every phase has its own MUCA weights and a small set of additional weights couple the different phases. As a method to determine in which phase the systems is, an loop update is presented. With typically less than  $L$  operations the information about all geometric loop lengths is obtained, given the loop lengths of the last configuration.

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The probability distribution  $P(m)$  for droplet configurations (solid) and strip configurations in  $X$  and  $Y$  direction (dashed) for an  $8 \times 8$  Ising system, at temperature  $T = 1.0$ , obtained with our new algorithm.

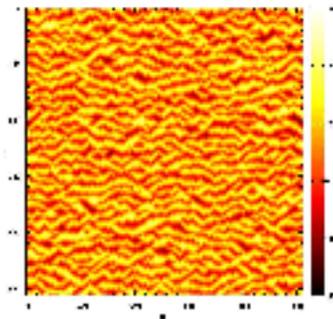
## P.41 Mapping two-dimensional surface patterns and scaling onto driven lattice gases

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We show that a  $(2+1)$ -dimensional discrete surface growth model exhibiting Kardar-Parisi-Zhang (KPZ) class scaling can be mapped onto a two-dimensional conserved lattice gas model of directed dimers. The KPZ height anisotropy in the surface model corresponds to a driven diffusive motion of the lattice gas dimers. We confirm by numerical simulations that the scaling exponents of the dimer model agree with those of the  $(2+1)$ -dimensional KPZ class. This suggests that the dimension dependence has a topological (exclusion) origin. The mapping opens up the possibility of analyzing growth models via reaction-diffusion models and allow much more efficient computer simulations (see [1]). In particular we provide very precise surface scaling exponents for  $d = 2, 3, 4, 5$  dimensions obtained by efficient bit-coded algorithms and discuss the problem of the debated upper-critical dimension of KPZ. Furthermore if we supplement this model with conserved, competing surface diffusion reactions we can obtain various, coarsening dot or ripple patterns (see image), which are important in self-organizing nano-structure research (see <http://www.iom-leipzig.de/for845/>).

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## P.42 Phase transitions in a coupled order parameter system on a scale-free network

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Models that display phase transitions with two coupled order parameters serve as archetypes to describe the phase behaviour in systems with several possible types of ordering. For example, a system may display both ferromagnetic and antiferromagnetic order with a coupling between the two. Others may show magnetic and superconducting, ferroelectric and ferromagnetic, or structural and magnetic order. These models are known for their rich phase diagrams and non-trivial critical behaviour. Here, we investigate the phase transitions of a corresponding model defined on a scale-free network. Besides the academic interest, this problem may have implications for models of opinion formation on social networks when opinions on different issues may be coupled, e.g. preferences for both a candidate and a political party.

Our analysis is based on thermodynamic arguments in the spirit of Landau theory, as suited for the description of phase transitions on scale free networks [1]. To add a microscopic background to the phenomenological approach we study a particular spin Hamiltonian that leads to coupled scalar order behaviour using the mean field approximation. Our results show [2] that the system is characterized by either of two types of ordering: either one of the two order parameters is zero or both are non-zero but have the same value. The critical behaviour of the model considered gives rise to non-trivial critical exponents, amplitude ratios and susceptibilities. While the critical exponents do not differ from those of a model with a single order parameter on a scale free network there are notable differences for the amplitude ratios and susceptibilities. Another peculiarity of the model is that the transverse susceptibility is divergent at all  $T < T_c$ , when  $O(n)$  symmetry is present. This behaviour is related to the appearance of Goldstone modes.

Acknowledgement: This work was supported by the Fonds zur Förderung der wissenschaftlichen Forschung under Project No. P19583-N20.

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## **P.43 Outbreak of epidemics in populations of morphologically complex hosts**

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Non-equilibrium phase-transitions between invading and non-invading regimes for epidemics in a spatial system of morphologically complex hosts defined on a lattice have been investigated numerically and analytically within the susceptible-infected-recovered (SIR) model. A quantitative link has been established between the host morphology and the features of epidemics in sets of morphologically realistic hosts such as neurons and plant roots. We have demonstrated that the invasion threshold is mainly determined by (i) the average overlap between neighbouring hosts, (ii) the morphological disorder, and (iii) the host shape anisotropy. Such an analysis allows simple morphological characteristics to be identified and used for epidemic outbreak analysis.

## **P.44 Spin-1 Heisenberg antiferromagnets with competing exchange and single-ion anisotropies**

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Using density matrix renormalization group calculations, ground state properties of the spin-1 Heisenberg chain with competing exchange and single-ion anisotropies in an external field are studied [1]. Our findings confirm and refine recent results [2] on the same model applying Monte Carlo techniques and perturbation theory. In particular, we present evidence for two types of biconical (or supersolid) and for two types of spin-flop (or superfluid) structures, in addition to the antiferromagnetic phase and the (10)-phase with magnetization plateau at half saturation [3]. The analysis is extended to two dimensions and finite temperatures by applying also Monte Carlo techniques. Basic features of the quantum phase diagrams are compared to related quantum and classical spin models [4, 5]. The research has been funded by the excellence initiative of the German federal and state governments.

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## **P.45 On the theory of word networks**

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Written human language is one of the most important examples of self-organization systems. Fundamental distributions of statistical mechanics for complex systems are derived from general principles; therefore, based on their grounds, the topology

description of the word network is of considerable interest. There are various algorithms for construction of a word networks. Our analysis show that topology of the word network depend on a way of construction. For the sake of concreteness, we shall consider two different algorithms for construction of word networks.

1. In terms of graph theory a finite chains correspond to separate sentences in our representation of the word network. At the network evolution, these finite chains intersect in the vertices that correspond to same words. We show, that in this case the topology of a network is described by  $q$ -exponent distribution function in the form

$$P(k) = \frac{(1 - (1 - q)\beta k)^{\frac{1}{1-q}}}{\sum_k (1 - (1 - q)\beta k)^{\frac{1}{1-q}}}. \quad (1)$$

2. A complete graph corresponds to separate sentences in our representation of the word network. At the network evolution, these complete graphs intersect in the vertices that correspond to same words. We show, that in this case the topology of a network is described by  $q$ -exponent distribution function in the form

$$P(k) = \frac{(1 - (1 - q)\beta(k - \kappa_0)^2)^{\frac{1}{1-q}}}{\sum_k (1 - (1 - q)\beta(k - \kappa_0)^2)^{\frac{1}{1-q}}}. \quad (2)$$

By maximizing the nonextensive entropy with the constraints we get the  $q$ -exponential functions defined by equations (1) and (2). We offer an analysis of the novels "The Sound and the Fury" by W. Faulkner in English and in Russian. Our special interest in the novel "The Sound and the Fury" by W. Faulkner was the fact that its four parts correspond to four types of perception; however, they are induced by the same events. Therefore, we have analyzed the corresponding parts of the novel and substantively constructed word networks that correspond to various types of perception. The first network (B) corresponds to the infant, pre-logic, sensuous perception of Benjamin, the second network (K) corresponds to the adolescent broken perception of Quentin, the third one (J) to the adult, pragmatic, unimaginative perception of Jason and the fourth network (A) corresponds to the wider and more independent perception of the author-observer. Besides, we have analyzed the word network (T) that corresponds to the novel on the whole. We have constructed degree distributions for each of the word networks and defined the value of the nonextensivity parameter  $q$  with the maximum likelihood method. We show that for different algorithms of construction of a network the values of nonextesivity parameters are various, but their ordering is invariant. Besides if the translation of the novel is regarded as mapping, the nonextensivity parameters ordering  $q_B > q_W > q_J > q_Q > q_A$  is an invariant of this mapping.

## P.46 The Cauchy problem for BBGKY hierarchy of quantum kinetic equations with coulomb potential

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In the work the Cauchy problem for BBGKY's hierarchy of quantum kinetic equations with coulomb potential is solved. By a semigroup method the existence of a unique solution of the BBGKY hierarchy of quantum kinetic equations in terms of initial data is proved.

## P.47 Dynamics of non-Abelian $Z_2$ spin vortices in frustrated spiral phase

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In magnetic phase of  $Nd$  doped  $La_{2-x}Sr_xCuO_4$  (LSCO) ( $0.02 < x < 0.04$ ) spins are ordered in spirals. Such spin configuration is caused by a magnetic dipole moment induced by a hole in antiferromagnetic background. A fraction of dipoles are well ferromagnetically ordered, in low temperature, forming, approximately, collinear, anisotropic superstructure [1]. A long range magnetic dipole interaction makes a spiral phase frustrated. In frustrated spiral phase the topological defects (TD)- non-Abelian  $Z_2$  vortices are present. TD are essential for a charge transport in LSCO, since charge carriers are attached to them. In this model of the cuprates conductivity the anisotropy of conductivity is induced by the anisotropy of magnetic phase; no translational symmetry of charge is violated, in agreement with experiment.

The relevant mobile (i.e. final energy (mass)) TD in frustrated spiral phase is  $Z_2$  vortex which interacts with frustrations. Representing frustrations by  $SO(3)$  gauge field the dynamics of  $Z_2$  vortex can be described by the  $SO(3)$  non-Abelian Higgs like model. We have derived the effective Hamiltonian of  $Z_2$  vortex and then quantize it. The resulting Hamiltonian describes heavy particle  $Z_2$  vortex which interacts with a bath of magnons and gauge field photons. The  $Z_2$  dynamics is reduced to

the quantum Brownian motion. The standard quantum kinetics methods allows us to evaluate the temperature dependence of the vortex damping coefficient and consequently the LSCO conductivity. The model where the basic mobile TD are pairs of  $Z_2$  vortices with opposite topological charge yields analogous results to ours [2].

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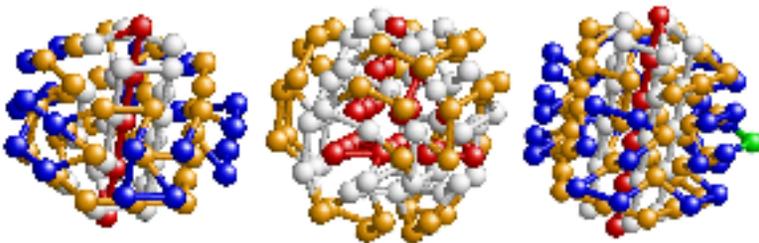
## P.48 Solid-solid transitions of flexible polymers

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Using multicanonical Monte Carlo methods we investigated a flexible elastic coarse-grained homopolymer model. We found wide similarities to the low-temperature behavior of atomic Lennard-Jones clusters including the dominance of icosahedral structures and multiple solid-solid transitions. In order to explore the narrow energy minima that belong to non-icosahedral conformations [1] we developed a new order parameter and modified the multicanonical simulation method. We were able to find decahedral, tetrahedral and fcc-like structures for polymers and atomic clusters and to investigate the associated solid-solid transitions.

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## P.49 Effect of disorder on equilibrium conformations of semiflexible polymers

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The structure and behaviour of biological cells is essentially affected by the biomechanical properties of semiflexible polymers. In the form of networks, such as the cytoskeleton, they build up the basic scaffold of eukaryotic cells. In order to study the mechanical properties of these highly complex systems, both interactions of the polymer with the surrounding network and further perturbing influences have to be taken into account. We investigate the equilibrium structure of semiflexible polymers in different potential landscapes by Monte Carlo simulations. In our simulations we use two approaches, a lattice and an off-lattice model. In the first, the polymer is represented by a self-avoiding walk on a lattice with defects that represent the disorder. In the second, the semiflexible polymer is described by a Heisenberg chain, a discretized wormlike chain model. Relevant observables such as the end-to-end distribution function and the tangent-tangent correlation function are discussed. The disorder potential is modeled according to the underlying experimental biological system.

## P.50 The critical Binder cumulant in two-dimensional Ising models

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We study two-dimensional Ising models on square and triangular lattices with isotropic and anisotropic interactions, using Monte Carlo simulations. The critical Binder cumulant,  $U^*$ , at the phase transition belonging, in all cases studied, to the 2d Ising universality class is found to depend on boundary condition, shape of the system, and anisotropy of the couplings (and thence anisotropy of critical spin correlations) [1, 2]. The fact that the transition temperature is exactly known in the considered models allows an accurate determination of  $U^*$ . We discuss the possibility of a

generic critical Binder cumulant by adjusting shape to anisotropy. Results are compared to findings by Chen and Dohm based on renormalization group calculations [3].

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## **P.51 Symmetries and dualities of random Ising ferromagnets**

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We study the critical behavior of  $d$ -dimensional random Ising ferromagnets with weak quenched disorder. In the critical region this model is known to be described by both the conventional Ginzburg-Landau Hamiltonian and the two-dimensional fermionic Gross-Neveu model in the  $n = 0$  limit. Renormalization group (RG) calculations are used to obtain the temperature dependences near the critical point of some thermodynamic quantities, the large distance behavior of the two-spin correlation function and the equation of state at criticality. It was shown that the Kramers-Wannier dual symmetry is the most powerful approach for receiving critical exponents in the two-dimensional dilute systems as well as numerical calculations in the  $d$ -dimensional case. At the present time there are two important questions of the theory of critical phenomena, these being the problem of a universality of the critical behavior of random systems and the role of Griffiths singularities.

## P.52 Increase of efficiency in interacting molecular motors

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We investigate the model of “reversible ratchet” with interacting particles. We calculate their energetic efficiency, when acting as molecular motors carrying a load against external force. It is shown that interaction between particles enhances the efficiency in wide range of parameters. We show that the effect has energetic, rather than entropic, origin. We also show complicated structures emerging in the interaction and density dependence of the current and response function. The fluctuation properties of the work and input energy indicate in detail the far-from-equilibrium nature of the dynamics. Besides the simulation results we show that a rather sophisticated mean-field-like approximation grasps well the phenomenon of the efficiency increase and yields further quantities, especially the non-Gaussian large-deviation function for work fluctuations. Possible consequences for artificial molecular motors are discussed.

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## P.53 Statistical mechanical description of liquid systems in electric field

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We formulate the statistical mechanical description of liquid systems for both polarizable and polar systems in an electric field in the  $\mathbf{E}$ -ensemble, which is the pendant to the thermodynamic description in terms of the free energy at constant potential. The contribution of the electric field to the configurational integral  $\tilde{Q}_N(\mathbf{E})$  in the  $\mathbf{E}$ -ensemble is given in an exact form as a factor in the integrand of  $\tilde{Q}_N(\mathbf{E})$ . We calculate the contribution of the electric field to the Ornstein-Zernike formula for the scattering function in the  $\mathbf{E}$ -ensemble. As an application we determine the field induced shift of the critical temperature for polarizable and polar liquids, and show

that the shift is upward for polarizable liquids and downward for polar liquids.

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## **P.54 Traffic flow of a mixture of cars with different properties**

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Statistical properties of traffic flow of a system consisting of two types of cars on a single-lane road are studied. The behaviour of cars is characterized by the probability distribution of car velocity as a function of headway and the velocity of the car ahead. Steady state properties of such a system are obtained by maximizing its entropy for given density and mean velocity of vehicles.

A similar system of identical cars was studied in [1] where phase transitions between free-flow and congested phase, and formation of platoons of cars were found. Here we study a random mixture of two types of cars differing by their maximum velocity or breaking ability.

Statistical properties of the system are manifested by distribution of total velocity and fluctuations of total length of a small group of cars in a system with given mean density and the ratio of different car numbers. The correlations between cars appear after subtraction of the distribution of the same group of uncorrelated cars.

The distributions for a mixture of cars differ from both pure systems substantially. A small admixture of slow cars to a system of fast cars have a dramatic effect, when headways and velocities of cars are even smaller than the ones in the pure system of slow cars. Similarly, a small number of cars with poor brakes in the system of cars with highly efficient brakes causes formation of platoons of higher density and smaller velocity than in a pure group of cars of low ability to decelerate.

The model is also generalized for possibility of input and output of cars to and from the lane at crossings.

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## P.55 Scaling of spin avalanches in growing networks

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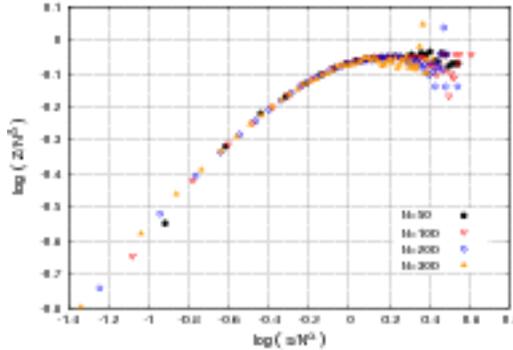
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Growing networks decorated with antiferromagnetically coupled spins are archetypal examples of complex systems due to the frustration and the multivalley character of their energy landscapes [1]. Here we use the damage spreading (DS) method [2] to investigate the cohesion of spin avalanches in the exponential networks and the scale-free networks. On the contrary to the conventional methods [3, 4], the results obtained from DS suggest that the avalanche spectra are characterized by the same statistics as the degree distribution in their home networks. Further, the obtained range  $Z$  of avalanches, i.e. the maximal distance reached from the damage, scales with the avalanche size  $s$  as

$$Z \propto N^\beta f(N^{-\alpha} s)$$

where  $\alpha \approx 0.5$  and  $\beta \approx 0.33$ . These values are true for both kinds of networks for the number  $M$  of nodes to which new nodes are attached between 4 and 10; a check for  $M=25$  confirms these values as well.

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[2] M. L. Rubio Puzzo and E. V. Albano, Commun. Comput. Phys. **4** (2008) 207.  
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Scaling in exponential networks of size  $N$ , where  $M = 5$ .

## P.56 Exact solution of a stochastic SIR model

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The susceptible-infectious-recovered (SIR) model describes the evolution of three species of individuals which are subject to an infection and recovery mechanism. A susceptible  $S$  can become infectious with an infection rate  $\beta$  by an infectious  $I$ -type provided that both are in contact. The  $I$ -type may recover with a rate  $\gamma$  and from then on stay immune. Due to the coupling between the different individuals, the model is nonlinear and out of equilibrium. We adopt a stochastic individual-based description where individuals are represented by nodes of a graph and contact is defined by the links of the graph. Mapping the underlying Master equation into a quantum formulation in terms of spin operators, the hierarchy of evolution equations can be solved exactly for arbitrary initial conditions on a linear chain. In case of uncorrelated random initial conditions the exact time evolution for all three individuals of the SIR model is given analytically. Depending on the initial conditions and reaction rates  $\beta$  and  $\gamma$ , the  $I$ -population may increase initially before decaying to zero. Due to fluctuations, isolated regions of susceptible individuals evolve and unlike in the standard mean-field SIR model one observes a finite stationary distribution of the  $S$ -type even for large population size. The exact results for the ensemble averaged population size are compared with simulations for single realizations of the

process and also with standard mean-field theory which is expected to be valid on large fully-connected graphs.

[1] G. M. Schütz, M. Brandau, and S. Trimper, Phys. Rev. E **78** (2008) 061132.

## **P.57 Counterions confined by charged nanosurfaces**

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It has been realized recently that nanotechnology is not just about nanoparticles; also nano-sized surfaces could play an important role and in some cases govern the behavior of nearby particles and molecules. In this report we present some theoretical and computer simulations results which show remarkable effects that can be produced by a charged nano-sized surface on the macroscopic behavior of nearby charged species, where the shape and size of the surface itself is equally or even more important than the direct interaction between the particles. The essence of our approach lies in exploiting the fact that nano-sized confinement is confinement of finite dimensions. The finite nature of nano-sized charged surface or just a nano-sized charged area on a larger surface leads to a non-zero electric potential gradient along the confinement.

In the case of charged planar surface the equilibrium position for a single counter-charge is above the center of the charged area. If more than one counter-charge is present, these charges compete for this equilibrium position and, at the same time, repel each other due to Coulomb interactions, which effectively leads to a rather stable equilibrium between particle-particle Coulomb repulsion and surface-induced Coulomb attraction due to the surface finiteness. We find that the like-charged particles, independent of their number, all become confined on the oppositely charged area if the surface charge balances the total charge carried by the particles. The local density of the particles above the charged area is not homogeneous; a higher particle density is found near the boundaries of the charged area with a clear tendency of layer formation along the area.

An extension of the finite confinement effect to cylindrical geometry helps to illustrate the principal forces that would govern the behavior of charged species in oppositely charged nanopores. We find that one of the consequences of a charged

pore wall is the aggregation of mobile charges in the pore with arrangements characteristic for different occupancies. Applications to study occupancy and valence selectivity in biological ion channels will be discussed.

## **P.58 Thickness-dependent secondary structure formation of tubelike polymers**

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By means of sophisticated Monte Carlo methods, we investigate the conformational phase diagram of a simple model for flexible polymers with explicit thickness [1, 2]. The thickness constraint, which is introduced geometrically via the global radius of curvature of a polymer conformation, accounts for the excluded volume of the polymer and induces cooperative effects supporting the formation of secondary structures [3]. In our detailed analysis of the temperature and thickness dependence of the conformational behavior for classes of short tubelike polymers, we find that known secondary-structure segments like helices and turns, but also ringlike conformations and stiff rods are dominant intrinsic topologies governing the phase behavior of such cooperative tubelike objects. This shows that the thickness constraint is indeed a fundamental physical parameter that allows for a classification of generic polymer classes.

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## **P.59 On thermodynamics and shape variation of lipid systems self-assembled in water solutions**

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Lipid molecules spontaneously form a number of unilamellar and multilamellar membrane structures of tubular or spherical shapes in water solutions. These closed lipid membrane shells (liposomes) are considered now as a convenient cell membrane model since it has its basic micromechanical and thermodynamic properties. Smallest lipid aggregates in fluids have a submicron size and demonstrate intensive Brownian motion in dispersions.

In this work we present our study on mechanics and thermodynamics of lipid aggregates both under the stress-free conditions and under the application of mechanical stress. First, we suggest a method of measuring Boltzmann's constant using video recorded motion of trapped lipid Brownian particles in such a liposome considered as a closed thermodynamic system at the absence of mechanical stress and provide this video and the results of measurements to the audience. Second, our study also includes a study of lipid tethers - long tubular membranes during the application of mechanical shear stress to the system. These tubular tethers demonstrate high level of thermal fluctuations of their contour, the experimental fact used for the measurement of bending moduli of the lipid membranes. We discuss the shape variations of the lipid membranes and stress relaxation in terms of curvature elasticity theory.

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## **P.60 Cross correlations in scaling analyses of phase transitions**

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Thermal or finite-size scaling analyses of importance sampling Monte Carlo computer simulations in the vicinity of phase transition points often combine different

estimates for the same quantity, such as a critical exponent, with the intent to reduce statistical fluctuations. We point out that the origin of such estimates in the same time series often results in pronounced cross correlations which are usually ignored even in high-precision studies, generically leading to significant underestimation of statistical fluctuations. We suggest to use a simple extension of the conventional analysis taking correlation effects into account, which leads to improved estimators with often substantially reduced statistical fluctuations at almost no extra cost in terms of computation time.

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## **P.61 Lattice model of liquid crystalline structures with spontaneously broken chiral symmetry**

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By molecular modeling we demonstrate that nematic long-range order (uniaxial and biaxial) discovered in bent-core liquid crystal systems reveals two further spatially homogeneous phases predicted by symmetry arguments [1]. The new phases are tetrahedratic nematic ( $T$ ) with  $D_{2d}$  symmetry and a chiral tetrahedratic nematic ( $N_T^*$ ) phase with  $D_2$  symmetry. These new phases were found for a lattice model with quadrupolar and octupolar anisotropic interactions using Mean Field theory and Monte Carlo simulations. Our results show that an interplay between quadrupolar and octupolar interactions stabilizes the new phases. To our knowledge, this is the first molecular model with spontaneous (homo-)chiral symmetry breaking in non-layered liquid crystals composed of bent-core molecules.

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## Frequently Asked Questions

**Who is the conference secretary?** Look for Ms. Lea Voigt.

**I am eligible for financial support, where do I get my money?** Just wait, the conference secretary Ms. Lea Voigt will contact you and inform you about the details.

**Is there a conference welcome?** On sunday evening, march 29 at 7:00 p.m. a welcome reception will take place in the roofed yard of the Insitute for Theoretical Physics, Vor dem Hospitaltore 1 (close to Ostplatz, see map on the back cover).

**Do you have WLAN access?** Certainly, it has the following parameters:

Wireless network (SSID):	UniLeipzig-Event
Network key (PSK):	Stat-Physics

The encryption protocol is WPA. The IP-addresses and the DNS server should be obtained automatically (DHCP). Please note that the network key (PSK) is **case sensitive**.

**I have no laptop, do you have computer rooms?** Sorry, there is no additional computer room available.

**There is this very important paper I want to read, do you have a printer?**

We will have a printer somewhere, if you really need to print something, ask Andreas Nußbaumer or Elmar Bitter for help.



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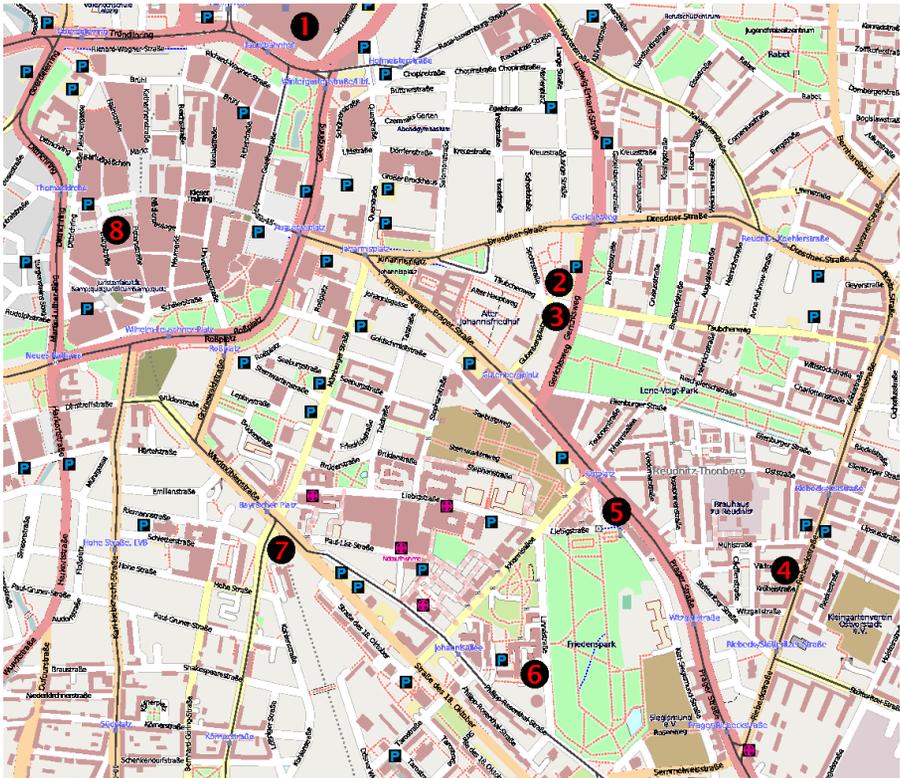
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## Time Table

	Monday	Tuesday	Wednesday
8:50 – 9:00	<i>Welcome</i>		
9:00 – 9:40	<b>Zia</b>	<b>Landau</b>	<b>Troyer</b>
9:40 – 10:00	Belyi	Hartmann	Cinti
10:00 – 10:20	Netočný	Paillusion	Wenzel
10:20 – 10:40	Topsøe	Vindigni	Berche
	<i>Coffee</i>	<i>Coffee</i>	<i>Coffee</i>
11:10 – 11:30	<b>Maret</b>	<b>Ahlers</b>	Nattermann
11:30 – 11:50			Parisen Toldin
11:50 – 12:10	Gomez-Solano	Folk	Kenna
12:10 – 12:30	Franosch	<i>Advisory board</i>	Fogedby
	<i>Lunch</i>	<i>Lunch</i>	<i>Lunch</i>
14:00 – 15:30	Poster	<i>Excursion</i>	Poster
15:30 – 16:10	<b>Löwen</b>		<b>Rácz</b>
16:10 – 16:30	Jug		Politi
16:30 – 16:50	Hsu		Usatenko
	<i>Coffee</i>		<i>Coffee</i>
17:20 – 18:00	<b>Redner</b>		<b>Kleinert</b>
18:00 – 18:20	Neri		<i>Closing</i>
18:20 – 18:40	Bock		
20:00	<i>Dinner</i>		<i>Dinner</i>

# Leipzig Map



- ❶ Main station
- ❷ Hotel Garni
- ❸ Hotel Tulip Inn
- ❹ Hotel Berlin
- ❺ Institute for Theoretical Physics (ITP), Vor dem Hospitaltore 1
- ❻ Lecture hall in the Physics Building, Linnéstr. 5
- ❼ Restaurant "Bayerischer Bahnhof"
- ❽ Restaurant "Thüringer Hof", Burgstr. 19