ABSTRACTS

of talks at the

6th NTZ-Workshop on

Computational Physics

CompPhys05

Institut für Theoretische Physik, Universität Leipzig, Germany

01 & 02 December 2005

http://www.physik.uni-leipzig.de/~janke/CompPhys05

Supported by the Centre for Theoretical Sciences (NTZ) of the Centre for Advanced Studies (ZHS) of Universität Leipzig, the EU-Marie Curie Development Host Grant No. IHP-HPMD-CT-2001-00108, EU-Marie Curie Network "ENRAGE": *Random Geometry and Random Matrices: From Quantum Gravity to Econophysics* under grant No. MRTN-CT-2004-005616, the PPP-Programme of the DAAD, and the Deutsche Forschungsgemeinschaft.

CompPhys05

6th NTZ-Workshop on Computational Physics

1 & 2 December 2005
12/1: 9:00–18:15
12/2: 9:00–20:00

Institut für Theoretische Physik
Universität Leipzig, Germany
Lecture Hall: „Kleiner Hörsaal"
Physics Building, Linnéstr. 5

Invited Speakers:

Michael Bachmann (Leipzig)
Bertrand Berche (Nancy)
Kurt Binder (Mainz)
Elmar Bittner (Leipzig)
Leszek Bogacz (Leipzig)
Zdzislaw Burda (Krakow)
Martino De Prato (Stuttgart)
Frank Dressel (Dresden)
Andrei Fedorenko (Halle)
Andrea Gambassi (Stuttgart)
Ulrich Hansmann (Jülich/Houghton)
Meik Hellmund (Leipzig)
Malte Henkel (Nancy)
Hsiao-Ping Hsu (Mainz)
Anders Irbäck (Lund)
Des Johnston (Edinburgh)
Dragi Karevski (Nancy)
Ralph Kenna (Coventry)
Klaus Kroy (Leipzig)
Harald Markum (Wien)
Thomas Michael (Halle)
Harald Morgner (Leipzig)
Thomas Neuhaus (Jülich)
Ricardo Paredes (Caracas)
Michel Pleimling (Erlangen)
Fabian Senf (Leipzig)
Semjon Stepanow (Halle)
Horst L. Vörtler (Leipzig)
Bartlomiej Waclaw (Krakow)
Martin Weigel (Edinburgh)

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Partially co-funded by the EU-Marie Curie Development Host Grant. No. IHP-HPMD-CT-2001-00108, the EU-Marie Curie Network „Enrage": *Random Geometry and Random Matrices: From Quantum Gravity to Econophysics* under grant No. MRTN-CT-2004-005616, the PPP-Programme of the DAAD, and the Deutsche Forschungsgemeinschaft.

Organizer: Wolfhard Janke, *CQT* group, ITP

CompPhys05 Timetable

December 01, 2005 - Linnestr. 5, Small Lecture Hall ("Kleiner Hörsaal")

09:00-09:15 **- Welcome Coffee -** 

Session 1: Phase Transitions and Critical Phenomena I (Chair: Kurt Binder)

09:15-09:40	**Malte Henkel**	Supersymmetric extensions of Schrödinger-invariance
09:40-10:05	**Ralph Kenna**	Scaling relations for logarithmic corrections
10:05-10:30	**Ricardo Paredes**	Three-dimensional Ising model confined in low-porosity aerogels: a Monte Carlo study
10:30-11:45	**Martino De Prato**	The critical Casimir effect in a slab geometry: a Monte Carlo study

10:45-11:15 **- Coffee Break -** 

Session 2: Protein Folding (Chair: Klaus Kroy)

11:15-11:40	**Anders Irbäck**	Thermal versus mechanical unfolding of ubiquitin
11:40-12:05	**Ulrich Hansmann**	All-atom protein simulations
12:05-12:20	**Frank Dressel**	Energy landscapes of proteins using the dynamical lattice model
12:20-12:35	**Michael Bachmann**	Conformational transitions of polymers and peptides near attractive substrates

12:35-14:30 **- Lunch Break at "Das Fass" (Johannisallee 20/Ostplatz) -** 

Session 3: Fluctuating Polymers (Chair: Anders Irbäck)

14:30-14:55	**Klaus Kroy**	How does a stretched polymer relax?
14:55-15:20	**Semjon Stepanow**	On the behaviour of short Kratky-Porod chain
15:20-15:35	**Hsiao-Ping Hsu**	Simulations of alternating copolymer brushes with chemically different side chains

Session 4: Posters (Chair: Des Johnston)

15:35-15:40	**Harald Markum**	Sonification of physical observables across phase transitions: from QCD to polymers (with on-line demonstrations during poster session)

15:40-16:00 **Short oral presentations of posters**

16:00-17:15 **- Poster Session & Coffee Break -** 

Session 5: Joint Faculty- and NTZ-Colloquium (Chair: Wolfhard Janke)

17:15-18:15	**Kurt Binder**	New interface-controlled phase transitions in nanosystems
19:00-20:30		**- Glühwein at Christmas Market -**
20:30		**- Dinner at "Thüringer Hof" -** 

December 02, 2005 - Linnestr. 5, Small Lecture Hall ("Kleiner Hörsaal")

09:00-09:15 **- Wake-Up Coffee -** 

Session 6: Disordered Systems (Chair: Malte Henkel)

09:15-09:40	**Bertrand Berche**	Influence of quenched dilution on the quasi-long-range ordered phase of the 2D XY model
09:40-09:55	**Elmar Bittner**	Free-energy barriers in a mean-field spin-glass model
09:55-10:10	**Martin Weigel**	Ground states and defect energies of the two-dimensional XY spin glass
10:10-10:25	**Meik Hellmund**	Series expansions for bond-diluted Ising models and percolation on Z^D
10:25-10:40	**Fabian Senf**	H-theorem for interacting systems driven by multiplicative noise
10:40-11:15		**- Coffee Break -** 

Session 7: Statistical Physics (Chair: Ulrich Hansmann)

11:15-11:40	**Harald Morgner**	Thermodynamic treatment of inhomogeneous and non-equilibrium systems
11:40-11:55	**Horst L. Vörtler**	Simulation of chemical potentials and phase equilibria of bulk and confined fluids by particle insertion methods
11:55-12:20	**Zdzislaw Burda**	Random matrices and risk management
12:20-12:35	**Bartlomiej Waclaw**	On simulating complex networks
12:35-14:30		**- Lunch Break at Pizzeria "Da Salvo" (Phillip-Rosenthal-Str. 9) -** 

Session 8: Phase Transitions and Critical Phenomena II (Chair: Bertrand Berche)

14:30-14:55	**Dragi Karevski**	Scaling and front dynamics in Ising quantum chains
14:55-15:10	**Leszek Bogacz**	Quantum Monte Carlo simulations of ferromagnetic chains
15:10-15:35	**Thomas Neuhaus**	A numerical study of the Meissner transition in the 3D FZS limit
15:35-15:50	**Thomas Michael**	Influence of layer defects in ferroelectric thin films
15:50-16:30		**- Coffee -** 

Session 9: Non-Equilibrium Thermodynamics (Chair: Ralph Kenna)

16:30-16:55	**Andrea Gambassi**	Critical behaviour of the two-dimensional randomly driven lattice gas
16:55-17:20	**Michel Pleimling**	Cluster dissolution and reentrance in time: surprises in the short-time critical dynamics
17:20-17:35	**Andrei Fedorenko**	Critical aging of a Heisenberg ferromagnet from a completely ordered state
17:35-18:00	**Des Johnston**	ASEPs, PASEPs, paths and (continued) fractions

18:00-20:00  **- Poster Session & Fare-Well Beer/Wine -** 

20:30 **- Dinner at ??? ("democratic decision") -**

December 03, 2005 - Vor dem Hospitaltore 1

Session 10:

10:00-17:00 **- Open Discussions of Project Groups -**

- Summary & Future Perspectives -

List of Posters in Session 4

Thierry Platini	Out of equilibrium process in quantum chains
Karsten Goede	Bindungsspezifität von Peptiden auf Halbleiteroberflächen
Gökhan Gökoglu	Structural properties of semiconductor binding synthetic peptides
Thomas Vogel	Coarse-grained polymer models: on-lattice vs. off-lattice
Simon Mitternacht	All-atom Monte Carlo simulations of ubiquitin unfolding
Andreas Nussbaumer	Evaporation/condensation of Ising droplets
Stefan Schnabel	Folding channels in coarse-grained heteropolymer models

List of Contributions

Michael Bachmann	Conformational transitions of polymers and peptides near attractive substrates
Bertrand Berche	Influence of quenched dilution on the quasi-long-range ordered phase of the 2D XY model
Kurt Binder	New interface-controlled phase transitions in nanosystems
Elmar Bittner	Free-energy barriers in a mean-field spin-glass model
Leszek Bogacz	Quantum Monte Carlo simulations of ferromagnetic chains
Zdzisław Burda	Random matrices and risk management
Martino De Prato	The critical Casimir effect in a slab geometry: a Monte Carlo study
Frank Dressel	Energy landscapes of proteins using the dynamical lattice model
Andrei Fedorenko	Critical aging of a Heisenberg ferromagnet from a completely ordered state
Andrea Gambassi	Critical behaviour of the two-dimensional randomly driven lattice gas
Karsten Goede	Bindungsspezifität von Peptiden auf Halbleiteroberflächen (P)
Gökhan Gökoglu	Structural properties of semiconductor binding synthetic peptides (P)
Ulrich Hansmann	All-atom protein simulations
Meik Hellmund	Series expansions for bond-diluted Ising models and percolation on $\mathbb{Z}^D$
Malte Henkel	Supersymmetric extensions of Schrödinger-invariance
Hsiao-Ping Hsu	Simulations of alternating copolymer bottle-brushes with chemically different side chains
Anders Irbäck	Thermal versus mechanical unfolding of ubiquitin
Desmond A. Johnston	ASEPs, PASEPs, paths and (continued) fractions
Dragi Karevski	Scaling and front dynamics in Ising quantum chains
Ralph Kenna	Scaling relations for logarithmic corrections
Klaus Kroy	How does a stretched polymer relax?
Harald Markum	Sonification of physical observables across phase transitions: from QCD to polymers
Thomas Michael	Influence of layer defects in ferroelectric thin films
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Harald Morgner	Thermodynamic treatment of inhomogeneous and non-equilibrium systems
Thomas Neuhaus	A numerical study of the Meissner transition in the 3D FZS limit
Andreas Nußbaumer	Evaporation/condensation of Ising droplets (P)
Ricardo Paredes	Three-dimensional Ising model confined in low-porosity aerogels: a Monte Carlo study
Thierry Platini	Out of equilibrium process in quantum chains (P)
Michel Pleimling	Cluster dissolution and reentrance in time: surprises in the short-time critical dynamics

Stefan Schnabel	Folding channels in coarse-grained heteropolymer models (P)
Fabian Senf	H-theorem for interacting systems driven by multiplicative noise
Semjon Stepanow	On the behaviour of short Kratky-Porod chain
Horst L. Vörtler	Simulation of chemical potentials and phase equilibria of bulk and confined fluids by particle insertion methods
Thomas Vogel	Coarse-grained polymer models: on-lattice vs. off-lattice (P)
Bartłomiej Wacław	On simulating complex networks
Martin Weigel	Ground states and defect energies of the two-dimensional XY spin glass

Conformational transitions of polymers and peptides near attractive substrates

Michael Bachmann

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The interest in understanding polymer adsorption at substrates has grown quite recently with the development of high-resolution experimental equipment allowing for studying the technologically important problem of substrate-binding specificity of synthetic peptides. In our study of simple hybrid models, we investigate how solubility of the surrounding solvent and temperature influence the substrate-binding of nongrafted polymers in a cavity with an attractive surface. Applying a suitably adapted variant of the multicanonical chain-growth algorithm for self-avoiding walks, we performed simulations of lattice polymers with up to 200 monomers and obtained the entire temperature-solubility pseudo-phase diagram of the hybrid system within a single simulation. We clearly separated expected thermodynamically stable phases dominated by the respective adsorbed and desorbed collapsed and random-coil conformations. Another central aspect of our study is the discussion of pseudo-phases that specifically depend on finite-size properties such as the precise number of monomers or, for peptides, the sequence of residues.

Influence of quenched dilution on the quasi-long-range ordered phase of the 2D XY model

Bertrand Berche

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The influence of non magnetic impurities in the 2D XY model is investigated through Monte Carlo (MC) simulations. The general picture of the transition is fully understood from the Harris criterion which predicts that the universality class is unchanged, and the Berezinskii-Kosterlitz-Thouless description of the topological transition remains valid. We nevertheless address here the question about the influence of dilution on the quasi-long-range order at low temperatures. In particular, we study the asymptotic of the pair correlation function and report the MC estimates for the critical exponent η at different dilutions. In the weak dilution region, our MC calculations are further supported by simple spin-wave-like calculations [see cond-mat/0309501].

New interface-controlled phase transitions in nanosystems

Kurt Binder

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Due to the current trend towards nanotechnology, the properties of systems "in between" bulk matter and single atoms and molecules become important. In a treatment of such systems in the framework of statistical mechanics, finite-size effects and surface effects become of utmost importance, as well as statistical fluctuations. Computer simulation is a very adequate tool to solve such tasks. These considerations are exemplified with studies of simple models where surface effects stabilize phase coexistence, and new types of phase transitions occur in special limiting cases. These phase transitions in a long cylinder or bipyramid geometry are related to wedge or cone filling transitions, and have unconventional critical behavior. Simulation results are interpreted by phenomenological extensions of finite-size scaling theory. The extent to which these phenomena can be observed in real systems will be briefly discussed.

Free-energy barriers in a mean-field spin-glass model

Elmar Bittner

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The mean-field Sherrington-Kirkpatrick spin-glass model is investigated by means of Monte Carlo simulations employing multioverlap and parallel tempering methods. We investigate the finite-size scaling behaviour of the free-energy barriers which are visible in the probability density of the Parisi overlap parameter. Assuming that the mean barrier height diverges with the number of spins N as N^α, our data show good agreement with the theoretical value $\alpha = 1/3$. We also found that the free-energy barriers of the Sherrington-Kirkpatrick spin-glass model are non-self-averaging and distributed according to the Fréchet extremal value distribution.

Quantum Monte Carlo simulations of ferromagnetic chains

Leszek Bogacz

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We use the Quantum Monte Carlo Stochastic Series Expansion (SSE) algorithm to investigate the properties of the one-dimensional Heisenberg ferromagnet. We consider the model for spins $s = 1/2$ or $s = 1$ and study the dependence of specific heat, magnetisation and magnetic susceptibility on temperature and magnetic field. Obtained results are compared to those received by analytical methods (Bethe ansatz, Green function, Random Phase Approximation).

Random matrices and risk management

Zdzisław Burda

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Asset allocation and portfolio theory are central issues in quantitative finance. In practice, the quality of the constructed portfolio depends on the quality of the estimator of the empirical covariance matrix for price changes of the assets on the market. We will describe a method of cleaning the empirical covariance matrix, which is based on random matrix theory. This method leads to a powerful computational tool in the problem of optimal portfolio construction [see http://xxx.lanl.gov/abs/cond-mat/0305627].

The critical Casimir effect in a slab geometry: a Monte Carlo study

Martino De Prato

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We consider a confined system undergoing a second-order phase transition. Criticality produces an effective interaction between the confining walls that is called the critical Casimir force. This force is given by a universal scaling function that depends on the boundary conditions. The force can be experimentally measured, for instance in binary liquid mixtures or Helium films. We introduce a method that enables to compute the Casimir force by means of Monte Carlo simulations of lattice models. We apply the method to the Ising class and study the resulting scaling functions.

Energy landscapes of proteins using the dynamical lattice model

Frank Dressel[1]
(with Sigismund Kobe[1] **and Michael Schroeder**[2]**)**

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Proteins are molecular machines in living cells. Their functions are largely dependent on their spatial structure. Therefore, the knowledge of protein folding pathways and structural changes is important to understand possible malfunction as Alzheimer disease or mucoviscidosis. Despite of the huge complexity of the problem, a simple model for structure prediction can be applied [1] to investigate the exact low-lying energy landscape of proteins. An introduction into the model is given and the energy landscapes for some small proteins (e.g. Trp-cage (1L2Y) and Cecropin-Magainin hybrid (1D9J)) are presented. The energy landscape will be discussed in terms of metastable states and competitions with the ground state.

References

[1] F. Dressel and S. Kobe, *Global optimization of proteins using a dynamical lattice model*, arXiv:q-bio.BM/0412031.

Critical aging of a Heisenberg ferromagnet from a completely ordered state

Andrei Fedorenko

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We adapt the non-linear σ model to study the nonequilibrium critical dynamics of $O(n)$ symmetric ferromagnetic system. Using the renormalization group analysis in $d = 2 + \epsilon$ dimensions we investigate the relaxation of the system starting from a completely ordered state. We find that the average magnetization obeys the long-time scaling behavior almost immediately after the system starts to evolve while the correlation and response functions demonstrate scaling behavior which is typical for aging phenomena. The corresponding fluctuation-dissipation ratio is computed to first order in ϵ and the relation between transverse and longitudinal fluctuations is discussed [see http://arxiv.org/abs/cond-mat/0507112].

Critical behavior of the two-dimensional randomly driven lattice gas

Andrea Gambassi

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The randomly driven lattice gas (RDLG) is a kinetic lattice gas model whose particles have a nearest-neighbour attractive interaction and, in addition, are driven along one of the lattice axes by an external field E with randomly changing sign. For $E = 0$ the model reduces to the standard equilibrium lattice gas and therefore, upon varying the temperature and for density 1/2, it undergoes a second-order phase transition belonging to the Ising universality class. Remarkably, the transition persists also for the non-equilibrium case of non-zero E, although it differs in nature from the equilibrium one. Recently, it has been argued that the RDLG has the same critical properties as the (non-equilibrium) driven lattice gas with constant drive (DLG), in contrast to the expectations based on the field-theoretical approach. With a suitable finite-size scaling (FSS) analysis of new Monte Carlo data we provide novel evidences that the DLG and RDLG have indeed different critical properties. The comparison of numerical data with finite-size scaling functions analytically computed within the field-theoretical approach fully support the standard picture of the phase transition in the RDLG

Bindungsspezifität von Peptiden auf Halbleiteroberflächen

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Structural properties of semiconductor binding synthetic peptides

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The determination of 3D structure of proteins and polypeptides has great importance due to their biological activities. In a newly growing area of research, synthetic peptides are used to build nano-devices due to their self-assembly and recognition properties. It is known that the binding of peptides on metal and semiconductor surfaces is strongly dependent of the amino acid sequences. In our study, we have analysed three 12-residue synthetic peptides, AQNPSDNNTHTH (S1), AQNPSDNNTATA (S2) and TNHDHSNAPTNQ (S3), whose binding properties were investigated in recent experimental studies. The second chain is a mutated version of the first one, and histidine residues of the first chain are replaced by alanines. The last chain is a randomly permuted sequence of the first chain. We have performed exhaustive multicanonical simulations of these peptides in order to investigate the thermodynamic and structural properties as well as the characteristic helix-coil transitions. Effects of solvation are also included by using an implicit solvent accessible surface area (ASA) model with OONS atomic solvation parameter set.

All-atom protein simulations

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The successful deciphering of the human genom has highlighted an old challenge in protein science: for most of the resolved protein sequences we do not know the corresponding structures and functions. Neither do we understand in detail the mechanism by which a protein folds into its biologically active form. Computer experiments offer one way to evaluate the sequence-structure relationship and the folding process. I will discuss various algorithms for this purpose in the context of simulations of small proteins (of size 30–60 residues). We study for these molecules the folding mechanism and the relation between secondary structure formation and folding. Limitations of current energy functions are discussed.

Series expansions for bond-diluted Ising models and percolation on $\mathbb{Z}^D$

Meik Hellmund

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We derive high-temperature series expansions for the free energy and the susceptibility of random-bond q-state Potts models on hypercubic lattices using a star-graph expansion technique.

For the case of the Ising ($q = 2$) model, disordered by quenched bond dilution, a detailed analysis of the influence of the disorder on the second-order phase transition (change in critical temperature and exponent γ) is presented for 3, 4 and 5 dimensions.

In the pure (no disorder) case we obtain series for the free energy and susceptibility with explicit q- and D-dependence up to order 17 (arbitrary D) and 19 ($D \leq 5$), resp. This allows us to analyze bond percolation ($q \to 1$) and tree percolation ($q \to 0$) and obtain critical exponents in various dimensions.

Supersymmetric extensions of Schrödinger-invariance

Malte Henkel

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The Levy-Leblond equation is the spin-1/2 analogue of the Schrödinger equation. By treating the non-relativistic 'mass' as a new variable, the solutions of the Levy-Leblond and Schrödinger equations form a supermultiplett and in 1D a dynamic supersymmetry isomorphic to OSp(4/2) is realized. This structure can be further clarified through isomophisms with certain Poisson algebras and allow for infinite-dimensional extensions of supersymmetric Schrödinger invariance (which include $N = 2$ Neveu-Schwarz theory). Applications to supercorrelation functions are described.

References

[1] M. Henkel and J. Unterberger, in preparation (2005).

Simulations of alternating copolymer bottle-brushes with chemically different side chains

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Single copolymer bottle-brushes consisting of two chemically different side chains grafted alternatively to straight rigid backbones are studied in three dimensions. They are described by self-avoiding random walks on a simple cubic lattice with and without nearest neighbour attractions between like monomers in a bad and a good solvent, respectively. We employ the pruned-enriched-Rosenbluth method (PERM) [1] to study this model with different repulsive interactions between unlike monomers, to understand the properties of the phase separation due to the incompatibility between chemically different side chains. The experimental evidence of the occurrence of the intramolecular phase separation for copolymacromonomers was given by Schmidt and co-workers [2]. With PERM, we have verified the existence of phase separation. But our preliminary results show that no phase transition occurs.

References

[1] P. Grassberger, Phys. Rev. E **56**, 3682 (1997).

[2] T. Stephan, S. Muth, and M. Schmidt, Macromolecules **35**, 9857 (2002).

Thermal versus mechanical unfolding of ubiquitin

Anders Irbäck

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The folding of the 76-residue protein ubiquitin has been extensively studied experimentally. Recently, the mechanical unfolding of this protein was studied by single-molecule constant-force techniques. Many observed unfolding traces had a simple two-state character, whereas others showed clear evidence of intermediate states. This talk presents an all-atom Monte Carlo study of the force-induced unfolding of ubiquitin. As in the experiments, the unfolding process is found to occur either in a single step or via intermediate states. One common feature can be identified in the simulated unfolding events, which is the order in which the secondary-structure elements break. The observed order remains to be verified experimentally and is not the same as in thermal unfolding at zero applied force, but appears physically reasonable.

ASEPs, PASEPs, paths and (continued) fractions

Desmond A. Johnston

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We note that a representation of the matrix algebra of the partially asymmetric exclusion process (PASEP,) a non-equilibrium model in 1D, lends itself to direct intepretation as the transfer matrix for 2D lattice paths, an equilibrium model. This allows a succint derivation of the normalisation of the PASEP, which is the equivalent of the partition function in equilibrium models. The correspondence means ideas that are applicable in the equilibrium context such as Lee-Yang zeros may also be deployed for the (P)ASEP

Scaling and front dynamics in Ising quantum chains

Dragi Karevski

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We study the relaxation dynamics of a quantum Ising chain initially prepared in a product of canonical states corresponding each to an equilibrium state of part of the chain at a given temperature. We focus our attention on the transverse magnetization for which a general expression is given. Explicit results are given for the completely factorized initial state, corresponding to a situation where all the spins are thermalized independently, and for the two-temperatures initial state, where part of the chain called the system is thermalized at a temperature T_s and the remaining part is at a temperature T_b.

Scaling relations for logarithmic corrections

Ralph Kenna

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Below the upper critical dimension, the universality class of a system is identified by its critical exponents and they obey the firmly-established scaling relations there. At the upper critical dimension, however, leading scaling behaviour is of the mean-field type and the universality class can instead be identified by the exponents of multiplicative logarithmic corrections to scaling. Corrections of this type also exist in other marginal scenarios. Here, scaling relations between the exponents of such logarithms are established and confronted with a variety of results from the literature.

How does a stretched polymer relax?

Klaus Kroy

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There are various ways to prepare a strongly (or even fully) stretched polymer. One may for example apply hydrodynamic flow, electric fields, pull at the ends, or – at least in theory and simulations – set the initial temperature to zero. Do these scenarios give rise to the same relaxation dynamics if the constraints are suddenly released? And how do the ends retract in time? Simple questions with controversial answers from theory, simulations, and experiments.

Sonification of physical observables across phase transitions: from QCD to polymers

Harald Markum[1]
(with Michael Bachmann[2], Alberto de Campo[3], Natascha Hörmann[1] and Wolfhard Janke[2])

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Sonification is defined as the use of non-speech audio to extract information from data and it represents the sound analogue to graphical visualization. The method is applied in several disciplines from economy to medicine to physics. Sonification might also help in analyzing critical phenomena. It could assist, together with graphical display, to examine the behavior of physical observables as a function of parameters like temperature, couplings and other variables of the system. In order to demonstrate the methodology for quantum chromodynamics (QCD) we analyzed the eigenvalues of the Dirac operator as a function of temperature from the confinement to the quark-gluon-plasma phase. An evaluation of data for the specific heat in the rich phase structure of polymers is devoted to the CompPhys05 Workshop. We are adapting program packages for audio browsing developed at the University of Graz within the interdisciplinary research project SonEnvir (http://sonenvir.at/).

Influence of layer defects in ferroelectric thin films

Thomas Michael

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Based on a modified Ising model in a transverse field we demonstrate that defect layers in ferroelectric thin films, originated by layers with impurities, vacancies or dislocations, are able to induce a strong increase or decrease of the polarization. The change is affected strongly by the variation of the exchange interaction within the defect layer. The applied Greens function method enables us to calculate the polarization, the excitation energy and the critical temperature of the material with structural defects.

All-atom Monte Carlo simulations of ubiquitin unfolding

Simon Mitternacht

Complex Systems Division, Dept. of Theoretical Physics, Lund University, Sweden
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We present results from all-atom Monte Carlo simulations of force-induced unfolding of the alpha/beta-protein ubiquitin. The same all-atom model has previously been used to study the folding of several peptides, as well as the aggregation of a fragment of the Alzheimer's Abeta peptide. The results for ubiquitin are consistent with data from single-molecule experiments, and provide details not accessible in the experiments. We also present some preliminary results from an ongoing study of thermal unfolding of ubiquitin, based on the same model.

Thermodynamic treatment of inhomogeneous and non-equilibrium systems

Harald Morgner

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Standard thermodynamics is designed to deal with homogeneous systems. In systems with more than one phase the relation between the phases is only a mathematical one while the explicit treatment of the physical interface between the phases is omitted. Consequently, standard thermodynamics is not suited to describe transport of matter between phases. As this process is of importance for industrial processes like liquid/liquid extraction various attempts have been made to overcome this situation. The naive approach, i.e., this simple application of the thermodynamic quantities to inhomogeneous systems can be shown to lead to inconsistent results. Two strategies can be distinguished in the literature. One approach is named after Cahn and Hilliard and remains within the continuum concept of matter. It introduces a correction term to the naive thermodynamic potential which is proportional to the second spatial derivative of the density. The other approach is the density functional method. It employs a concept from the atomic picture of matter, namely the interaction potential, to compute the potential energy. The present treatment starts with a naive concept, replacing the actual local density by a convoluted density without assigning a physical meaning to the convolution function in the first place. It turns out that this approach is suited to derive both other methods as special cases. The convoluting function exhibits close relation to the interaction potential of the density functional method. Further, is appears possible to derive the convolution function from conventional experimental data like molar volume, pressure and surface tension. Even though the convolution function is derived from equilibrium data the scheme is applicable to non-equilibrium systems as well.

A numerical study of the Meissner transition in the 3D FZS limit

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Using Worm updates, we study the 3D Meissner transition at finite magnetic field in the Frozen Superconductor Limit. The transition is expected to be related to 2D Bose Einstein condensation. We observe quite unusual finite-size effects in first preliminary simulations.

Evaporation/condensation of Ising droplets

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In [1] Kotecký *et al.* study the behaviour of finite-volume liquid-vapour systems at a fixed excess δN of particles above ambient gas density. They identify a dimensionless parameter $\Delta(\delta N)$ and a universal constant $\Delta_c(d)$ and show that for $\Delta < \Delta_c$ a droplet of the dense phase occurs while for $\Delta > \Delta_c$ the excess is absorbed in the background. The fraction λ_Δ of excess particles forming the droplet is given explicitly. Furthermore, they state, that the same is true for solid-gas systems.

To verify these results, we have simulated the spin-1/2 Ising model on a square lattice at constant magnetisation equivalent to a fixed particle excess in the lattice-gas picture. We measured the largest minority droplet, corresponding to the solid phase, at various system sizes ($L = 40, \ldots, 640$). Using analytic values for the spontaneous magnetisation m_0, the susceptibility χ and interfacial free energy τ_W for the infinite system, we were able to determine λ_Δ in very good agreement with the theoretical prediction. The measurements were repeated on a triangular lattice and for the next-nearest neighbour interaction giving similar good results.

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Three-dimensional Ising model confined in low-porosity aerogels: a Monte Carlo study

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The influence of correlated impurities on the critical behaviour of the 3D Ising model is studied using Monte Carlo simulations. Spins are confined into the pores of simulated aerogels (diffusion limited cluster-cluster aggregation) in order to study the effect of quenched disorder on the critical behaviour of this magnetic system. Finite size scaling is used to estimate critical couplings and exponents. A new universality class is found, although critical exponents seem close to those of the randomly diluted Ising model. The influence of correlated disorder, observed in effective exponents, is not observable at the corresponding asymptotic values.

Out of equilibrium process in quantum chains

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Cluster dissolution and reentrance in time: surprises in the short-time critical dynamics

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In nonequilibrium critical dynamics the system under consideration is prepared in some initial state from which it is quenched to the critical temperature and then let to evolve in time according to the given dynamical rules. Generally one is interested in the relaxation of the magnetization and in the behavior of the autocorrelation function. In most of the studied cases the initial state is of two kinds: it is either the (completely) ordered one or the (completely) disordered one. In this talk I show that an intriguing reentrance in time is encountered in critical relaxation measurements which start from a non-trivial initial state given by a ground state of the random field Ising model. Competition between two different mechanisms, the cluster dissolution of the compact cells and the usual domain growth, is responsible for this novel feature in nonequilibrium critical dynamics.

Folding channels in coarse-grained heteropolymer models

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H-theorem for interacting systems driven by multiplicative noise

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The H-theorem for a system of N globally coupled Stratonovich models is found and the convergence to the stationary solution independent of the initial distribution is proved. Due to the multiplicative noise and the interaction between the particles there is no detailled balance and therefore an analytical expression for the stationary distribution is not easily found. Nevertheless, the information contained in the system of coupled Langevin equations provides important hints to the qualitative structure of the stationary state. The state space of the stochastic motion is divided in sectors whose topology depends on the system parameters. The Langevin flow between these sectors can be determined. For large times the system is found with probability one in one of those sectors which have their boundary flows pointing inward, only. These are the ergodic components. This result is independent of the system size so that phase transitions associated with the breaking of ergodicity exist already for finite N. The critical exponent characterizing the order parameter near the critical point depends on all parameters of the Stratonovich model including the system size N if the latter is finite, for $N \to \infty$ see [1].

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On the behaviour of short Kratky-Porod chain

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Using the exact computation of a large number of moments of the distribution function of the end-to-end distance $G(r, N)$ of the worm-like chain, we have established the analytical form of the coefficients in Taylor expansions of the moments for short chain lengths N. The knowledge of these coefficients enabled us to resummate the moment expansion of $G(r, N)$ by taking into account consecutively the deviations of the moments from their stiff rod limit. Within this procedure we have derived the short-chain expansion for $G(r, N)$, the scattering function, and the extension-force relation, which take into account the deviations of the moments from their stiff rod limit to the seventh order in N.

Simulation of chemical potentials and phase equilibria of bulk and confined fluids by particle insertion methods

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We study chemical potentials and phase equilibria in dense bulk and confined fluid phases by means of particle insertion simulation methods. Since the classical Widom test particle method usually fails for dense complex fluids we have implemented several more recent insertion approaches, such as, a gradual particle insertion method [1] and several variants of a 'bonded/unbonded' particle insertion method [2]. Simulations of chemical potentials of highly associating primitive water models by means of these methods show the applicability of sophisticated particle insertion methods to network-forming fluid phases [3]. To study phase equilibria we simulate chemical potential versus density isotherms on subcritical temperatures and estimate the vapour-liquid equilibrium densities by applying an Maxwell equal area rule which we proposed some time ago [4]. In this paper we extend our studies to fluids confined to thin planar films including 2-dimensional arrangements. We study the properties of chemical potential vs. density isotherms and phase equilibria for both simple square-well fluids and primitive water models on bulk conditions and under confinement. Preliminary results show qualitative similar properties of chemical potential isotherms for the fluids under considerations on bulk and confined conditions and a general shift of the critical point to lower temperatures under confinement.

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Coarse-grained polymer models: on-lattice vs. off-lattice

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We investigated coarse-grained polymer models such as the HP on-lattice and the AB off-lattice formulations for heteropolymers ("proteins"). The poster will focus on the results of two problems. Firstly, we will give results of investigations concerning *designing sequences* in the HP model on lattices. To this end, we perform exact enumerations of the whole sequence-conformation space of HP proteins on the fcc lattice up to a certain chain length and compare with results from the simple cubic lattice. Secondly we try to show how "far" lattice models are from "reality", or from similar off-lattice models, respectively. Therefore we simulate off-lattice AB model-like proteins with different potentials and compare putative ground states with those from on-lattice simulations.

On simulating complex networks

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Two methods for simulating complex networks will be presented and some similarities as well as differences between resulting networks will be given.

Ground states and defect energies of the two-dimensional XY spin glass

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Considerable advances have been made in recent years in the understanding of Ising spin glass models in two and three dimensions. Models with continuous degrees-of-freedom, which are often more realistic in describing physical systems, have received much less attention. To make progress in this direction, the two-dimensional XY spin-glass model with bimodal coupling distribution is investigated by applying a novel "embedded matching" technique augmented by a specially tailored genetic algorithm to find numerically exact ground-state configurations for relatively large systems of up to 28×28 spins. Perhaps surprisingly, the resulting ground states are found to be non-generate, implying a critical exponent $\eta = 0$. The spin-glass phase at zero temperature is described by the scaling of the spin stiffness as determined from the energy differences between ground states of systems with different boundary conditions. Owned to the novel technique and the consequently larger accessible system sizes as well as elaborate finite-size scaling techniques, the corresponding spin-stiffness exponent θ_s is for the first time determined consistently from different sets of boundary conditions. Considering the stiffness of the system towards *chiral* excitations, a result different from the spin stiffness is found, strongly indicating the presence of spin-chirality decoupling [see cond-mat/0510614].

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