ABSTRACTS

of contributions to the

7th NTZ-Workshop on

Computational Physics

CompPhys06

Institut für Theoretische Physik, Universität Leipzig, Germany

30 Nov – 02 Dec 2006

http://www.physik.uni-leipzig.de/~janke/CompPhys06

Supported by the Centre for Theoretical Sciences (NTZ) of the Centre for Advanced Study (ZHS) of Universität Leipzig, 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 Alexander von Humboldt Foundation, the PPP Collaborative Research Programme of the DAAD, and the Deutsche Forschungsgemeinschaft.

CompPhys06

7th NTZ-Workshop on Computational Physics

30 November – 2 December 2006
11/30: 9:00–18:15
12/1: 9:00–20:00

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

Invited Speakers:

Michael Bachmann (Lund)
Piotr Bialas (Krakow)
Elmar Bittner (Leipzig)
Viktoria Blavatska (Leipzig)
Zdzislaw Burda (Krakow)
Christophe Chatelain (Nancy)
Volker Dohm (Aachen)
Andrei Fedorenko (Paris)
Martin Hasenbusch (Pisa)
Hsiao-Ping Hsu (Mainz)
Ferenc Iglói (Budapest)
Anders Irbäck (Lund)
Des Johnston (Edinburgh)
Dragi Karevski (Nancy)
Ralph Kenna (Coventry)
Harald Markum (Wien)
Oliver Melchert (Göttingen)
Thomas Neuhaus (Jülich)
Andreas Nußbaumer (Leipzig)
Holger Perlt (Leipzig)
Thierry Platini (Nancy)
Janett Prehl (Chemnitz)
Adriaan Schakel (Berlin)
Holger Schmidtchen (Leipzig)
Michael Schreiber (Chemnitz)
Lev Shchur (Moscow)
Semjon Stepanow (Halle)
Steffen Trimper (Halle)
Christian von Ferber (Coventry)
Horst Vörtler (Leipzig)
Bartlomiej Waclaw (Leipzig)
Martin Weigel (Edinburgh)

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Organizer: Wolfhard Janke, *CQT* group, ITP

CompPhys06 Timetable

November 30, 2006 - Linnéstr. 5, Small Lecture Hall ("Kleiner Hörsaal")

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

Session 1: Phase Transitions and Critical Phenomena I (Chair: Volker Dohm)

09:15-09:40	**Ralph Kenna**	Scaling theory for logarithmic-correction exponents
09:40-10:05	**Dragi Karevski**	Gradient critical phenomena in Ising quantum chain
10:05-10:30	**Christophe Chatelain**	Jarzynski relation and some applications
10:30-11:45	**Horst L. Vörtler**	System size dependence of chemical potentials and phase equilibria of bulk fluids and thin fluid films
10:45-11:15		**- Coffee Break -** 

Session 2: Proteins and Polymers (Chair: Klaus Kroy)

11:15-11:40	**Anders Irbäck**	Peptide folding and aggregation
11:40-11:55	**Michael Bachmann**	Mesoscopic modeling of protein folding and aggregation
11:55-12:20	**Hsiao-Ping Hsu**	What is the order of 2d escape transition?
12:20-12:35	**Semjon Stepanow**	Surface segregation of conformationally asymmetric polymer blends
12:35-14:30		**- Lunch Break at "Das Fass" (Johannisallee 20/Ostplatz) -** 

Session 3: Phase Transitions and Critical Phenomena II (Chair: Anders Irbäck)

14:30-14:55	**Thomas Neuhaus**	Tube picture of polymers
14:55-15:20	**Martin Hasenbusch**	The fully frustrated XY model in two dimensions
15:20-15:35	**Elmar Bittner**	Droplet condensation/evaporation transition

Session 4: Posters (Chair: Desmond Johnston)

15:35-16:00 **Short oral presentations of posters**

16:00-17:15 **- Poster Session & Coffee Break in the "Aula" -** 

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

17:15-18:15	**Volker Dohm**	Universality and diversity of critical phenomena
19:00-20:15		**- Glühwein at Christmas Market -**
20:30-		**- Dinner at "Thüringer Hof" (Burgstraße 19) -** 

December 1, 2006 - Linnéstr. 5, Small Lecture Hall ("Kleiner Hörsaal")

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

Session 6: Disordered Systems (Chair: Michael Schreiber)

09:15-09:40	**Ferenc Iglói**	Critical and tricritical singularities of the three-dimensional random-bond Potts model for large q
09:40-10:05	**Andrei Fedorenko**	Statics and dynamics of elastic manifolds in media with long-range correlated disorder
10:05-10:20	**Janett Prehl**	Diffusion on disordered fractals
10:20-10:35	**Viktoria Blavatska**	Self-avoiding walks on fractals: Scaling laws
10:35-10:50	**Oliver Melchert**	Fractal dimension of domain walls in two-dimensional Ising spin glasses

10:50-11:15 **- Coffee Break -** 

Session 7: Random Networks and Graphs (Chair: Ferenc Iglói)

11:15-11:40	**Martin Weigel**	Frustration from fat graphs
11:40-11:55	**Piotr Bialas**	Connected random graphs
11:55-12:10	**Bartlomiej Waclaw**	Networks interacting with matter
12:10-12:25	**Holger Schmidtchen**	Architecture of randomly evolving idiotypic networks
12:25-12:40	**Christian von Ferber**	Network dynamics: Laplacian of graphs and their local and global topology

12:40-14:30 **- Lunch Break at Pizzeria "Da Salvo" (Phillip-Rosenthal-Str. 9) -** 

Session 8: Dynamics and Non-Equilibrium Thermodynamics (Chair: Adriaan Schakel)

14:30-14:55	**Michael Schreiber**	Coherent destruction of the current through molecular wires using short laser pulse
14:55-15:10	**Des Johnston**	Continued fractions and the ASEP
15:10-15:25	**Steffen Trimper**	Master equation and two heat reservoirs
15:25-15:40	**Thierry Platini**	Diffusion of the transverse magnetization profil in quantum spin chains
15:40-15:55	**Holger Perlt**	Operator product expansion on the lattice: Analytic Wilson coefficients

15:55-16:30 **- Coffee Break -** 

Session 9: Statistical Physics (Chair: Ralph Kenna)

16:30-16:55	**Adriaan Schakel**	Spacetime approach to phase transitions
16:55-17:20	**Lev Shchur**	Harmonic measure probing of DLA clusters
17:20-17:45	**Zdzislaw Burda**	Random Levy matrices
17:45-18:00	**Andreas Nußbaumer**	Football fever: Goal distributions in football
18:00-18:15	**Harald Markum**	Fun with computational physics: Non-commutative geometry on the lattice

18:15-20:00  **- Poster Session & Fare-Well Beer/Wine -** 

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

December 2, 2006 - Vor dem Hospitaltore 1, Large ("Grosser") Seminar Room 1L12/13

Session 10: Computational Physics (Chair: Wolfhard Janke)

10:00-12:30	**- Open Discussions of Project Groups -**
12:30-14:30	**- Lunch Break at "Das Fass" (Johannisallee 20/Ostplatz) -**
14:30-17:00	**- Collaboration Meetings -**
17:00-18:00	**- Summary & Future Perspectives -**

List of Posters in Session 4

Frank Dressel	Coarse graining in protein models
Meik Hellmund	Series expansions for percolation and bond-diluted Ising models on Z^D
Martin Holtschneider	Anisotropic Heisenberg antiferromagnet in two dimensions
Christoph Junghans	Microcanonical analysis of polymer aggregation
Norio Kikuchi	Theory of DNA condensation
Daniel Rings	Simulation of shear-driven aggregation
Stefan Schnabel	Solution behavior of semiconductor-binding peptides
Thomas Vogel	Collapse and freezing transitions of polymers on regular lattices
Sandro Wenzel	Percolation of vortex networks in the U(1) lattice Higgs model
Stefan Wolfsheimer	Rare-event sampling in local sequence alignments
Stephan Zschiegner	Surface diffusion in potential landscapes

List of Contributions

Michael Bachmann	Mesoscopic modeling of protein folding and aggregation
Piotr Bialas	Connected random graphs
Elmar Bittner	Droplet condensation/evaporation transition
Viktoria Blavatska	Self-avoiding walks on fractals: Scaling laws
Zdzisław Burda	Random Levy matrices
Christophe Chatelain	Jarzynski relation and some applications
Volker Dohm	Universality and diversity of critical phenomena
Frank Dressel	Coarse graining in protein models (P)
Andrei Fedorenko	Statics and dynamics of elastic manifolds in media with long-range correlated disorder
Martin Hasenbusch	The fully frustrated XY model in two dimensions
Meik Hellmund	Series expansions for percolation and bond-diluted Ising models on $\mathbb{Z}^D$ (P)
Martin Holtschneider	Anisotropic Heisenberg antiferromagnet in two dimensions (P)
Hsiao-Ping Hsu	What is the order of 2d escape transition?
Ferenc Iglói	Critical and tricritical singularities of the three-dimensional random-bond Potts model for large q
Anders Irbäck	Peptide folding and aggregation
Desmond A. Johnston	Continued fractions and the ASEP
Christoph Junghans	Microcanonical analysis of polymer aggregation (P)
Dragi Karevski	Gradient critical phenomena in Ising quantum chain
Ralph Kenna	Scaling theory for logarithmic-correction exponents
Norio Kikuchi	Theory of DNA condensation (P)
Harald Markum	Fun with computational physics: Non-commutative geometry on the lattice
Oliver Melchert	Fractal dimension of domain walls in two-dimensional Ising spin glasses
Thomas Neuhaus	Tube picture of polymers
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Martin Weigel	Frustration from fat graphs
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Stefan Wolfsheimer	Rare-event sampling in local sequence alignments (P)
Stephan Zschiegner	Surface diffusion in potential landscapes (P)

Mesoscopic modeling of protein folding and aggregation

Michael Bachmann

Computational Biology and Biological Physics, Lund University, Sweden, and
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In this talk, the importance of mesoscopic models for soft materials is illustrated for folding processes of protein-like heteropolymers and their aggregation. In addition, it is shown that the conformational transitions accompanying folding and aggregation processes of naturally finite systems are similar to phase transitions, but not in a strict thermodynamic sense. In particular, the aggregation studies reveal the advantages of a microcanonical analysis, compared to the standard canonical approach.

Connected random graphs

Piotr Bialas

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In this contribution I will present calculations of the properties of the giant component in random graphs with given degree distribution. From this properties of the connected random graphs will be infered.

Droplet condensation/evaporation transition

Elmar Bittner

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We performed Monte Carlo simulations of the Ising model with nearest-neighbour couplings on a square lattice with periodic boundary conditions at fixed magnetisation and measured the largest minority droplet to confirm the analytical asymptotic results of Biskup *et al.* [*Europhys. Lett.* **60** (2002) 21] and to explore finite-size corrections not studied there.

Self-avoiding walks on fractals: Scaling laws

Viktoria Blavatska

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The scaling behavior of linear polymers in disordered media, modelled by self-avoiding random walks (SAWs) on the backbone of three- and four-dimensional percolation clusters is studied by Monte Carlo simulations. We apply the pruned-enriched Rosenbluth chain-growth method (PERM). Our numerical results bring about the estimates of critical exponents, which characterize disorder averages of end-to-end distance and number of SAWs.

Random Levy matrices

Zdzisław Burda

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Random matrices play an important role in many areas of research. Random matrices belonging to the Gaussian universality class have been extensively studied in the past. I will discuss non-Gaussian matrices belonging to the Levy universality class characterised by heavy tails in the probability distribution of matrix elements. One encounters such matrices for example in financial markets. Theory of heavy-tailed matrices is still in a very early stage. I will discuss spectral properties of Levy-Wigner matrices and of free random Levy matrices. Both the ensembles are the most important in the Levy universality class because they are stable with respect to matrix addition [cond-mat/0602087].

Jarzynski relation and some applications

Christophe Chatelain

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We will discuss the Jarzynski relation and its potential use in the context of spin systems. Monte Carlo calculation of critical exponents and order-order interface tension will be presented.

Universality and diversity of critical phenomena

Volker Dohm

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Critical phenomena are divided into so-called "universality classes" characterized only by the dimension d of the system and the number n of components of the order parameter. A prominent example is the ($d = 3$, $n = 2$) universality class of the superfluid transition of ^{4}He and of XY spin models. Several experiments under microgravity conditions supported by NASA are discussed that are designed to test the universality predictions of the renormalization-group theory. Another important universality class is the ($d = 3$, $n = 1$) case: ordinary fluids and uniaxial magnets. Within a given universality class, critical phenomena have recently been predicted to exhibit a considerable diversity due to van der Waals interactions and anisotropy effects. The latter violate the so-called "two-scale factor universality". Analytic predictions of nonuniversal anisotropy effects near T_c are presented that can be tested by Monte Carlo simulations for anisotropic Ising and XY models.

Coarse graining in protein models

Frank Dressel[1]
(with S. Kobe[1] and M. Schroeder[2])

Technische Universität Dresden: [1] Institut für Theoretische Physik, [2] Biotechnologisches Zentrum, 01062 Dresden
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Coarse graining is inherent in models for predicting protein tertiary structure from the sequence of amino acids. Such a model includes on the one hand coarse graining in structural space and on the other hand, coarse graining in the energy function is used. Here we present an approach to deal with this problem. Aspects of the structural coarse graining and that with respect to energy functions are discussed. Within the presented model, we are able to calculate the complete low-lying energy landscape for proteins up to 60 amino acids.

Statics and dynamics of elastic manifolds in media with long-range correlated disorder

Andrei Fedorenko

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We study the statics and dynamics of an elastic manifold in a disordered medium with quenched defects correlated as r^{-a} for large separation r. We derive the functional renormalization group equations to one-loop order which allow to describe the universal properties of the system in equilibrium and at the depinning transition. Using a double $\epsilon = 4 - d$ and $\delta = 4 - a$ expansion we compute the fixed points characterizing different universality classes and analyze their regions of stability. The long-range disorder-correlator remains analytic but generates short-range disorder whose correlator exhibits the usual cusp. The critical exponents and universal amplitudes are computed to first order in ϵ and δ at the fixed points. At depinning a velocity-versus-force exponent β larger than unity can occur. We discuss possible realizations using extended defects [cond-mat/0609234].

The fully frustrated XY model in two dimensions

Martin Herbert Hasenbusch

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We study the phase diagram and critical behavior of the two-dimensional square-lattice fully frustrated XY model (FFXY) and of two related models, a lattice discretization of the Landau-Ginzburg-Wilson Hamiltonian for the critical modes of the FFXY model, and a coupled Ising-XY model. We present a finite-size-scaling analysis of the results of high-precision Monte Carlo simulations on square lattices $L \times L$, up to $L = \mathrm{O}(10^3)$. In the FFXY model and in the other models, when the transitions are continuous, there are two very close but separate transitions. There is an Ising chiral transition characterized by the onset of chiral long-range order while spins remain paramagnetic. Then, as temperature decreases, the systems undergo a Kosterlitz-Thouless spin transition to a phase with quasi-long-range order. The FFXY model and the other models in a rather large parameter region show a crossover behavior at the chiral and spin transitions that is universal to some extent. We conjecture that this universal behavior is due to a multicritical point [cond-mat/0509682].

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

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.

Anisotropic Heisenberg antiferromagnet in two dimensions

Martin Holtschneider

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Heisenberg antiferromagnets with an uniaxial anisotropy in two dimensions have attracted much interest, both theoretically and experimentally. In particular, when applying an external field parallel to the easy axis, one obtains an interesting phase diagram, with an algebraically ordered spin-flop phase, in addition to the long-range ordered antiferromagnetic and the paramagnetic phases. In this poster, recent results on the classical and the quantum, $S = 1/2$, version of the model are presented, as have been found using Monte Carlo techniques. The work has been performed in cooperation with S. Wessel (Univ. Stuttgart), R. Leidl (Simon Fraser University), and W. Selke (RWTH Aachen) [Phys. Rev. B72 (2005) 064443].

What is the order of 2d escape transition?

Hsiao-Ping Hsu
(with Kurt Binder, Leonid I. Klushin, and Alexander M. Skvortsov)

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Grafted single polymers confined between two pistons are studied by Monte Carlo simulations using the PERM algorithm. They are described by N-step self-avoiding random walks on a square lattice between two parallel hard walls with distance H. As H decreases the chain is compressed uniformly and undergoes a phase transition beyond a certain critical compression force. One part of the chain forms a "stem" stretching from the grafting point to the edge of the piston, while the rest of the segments form a coiled "crown" outside the piston. It is unclear what is the order of 2d escape transition. In order to clarify this problem, we discuss the escape transition based on the blob picture and the Landau theory with the same order parameter defined for the ideal chain. The cross-over scaling behaviors of the free energy, compression force, and the order parameter are estimated from the simulations and compared to theoretical predictions.

Critical and tricritical singularities of the three-dimensional random-bond Potts model for large q

Ferenc Iglói

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We study the effect of varying strength δ of bond randomness on the phase transition of the three-dimensional Potts model for large q. The cooperative behavior of the system is determined by large correlated domains in which the spins point in the same direction. These domains have a finite extent in the disordered phase. In the ordered phase there is a percolating cluster of correlated spins. For a sufficiently large disorder $\delta > \delta_t$ this percolating cluster coexists with a percolating cluster of noncorrelated spins. Such a coexistence is only possible in more than two dimensions. We argue and check numerically that δ_t is the tricritical disorder, which separates the first- and second-order transition regimes. The tricritical

exponents are estimated as $\beta_t/\nu_t = 0.10(2)$ and $\nu_t = 0.67(4)$. We claim these exponents are q independent for sufficiently large q. In the second-order transition regime the critical exponents $\beta/\nu = 0.60(2)$ and $\nu = 0.73(1)$ are independent of the strength of disorder.

Peptide folding and aggregation

Anders Irbäck

Complex Systems Division, Department of Theoretical Physics, Lund University, Sweden

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All-atom Monte Carlo studies of peptide folding and aggregation based on a novel protein model with a simplified energy function are presented. We have previously demonstrated that this model gives a good description of the structure and thermodynamics of several well characterized sequences with about 20 amino acids. Recently, we used the same model to investigate structural differences between four semiconductor-binding peptides with 12 amino acids, whose adhesion properties to GaAs and Si surfaces have been studied by Goede *et al.*

Continued fractions and the ASEP

Desmond A. Johnston

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A tridiagonal matrix representation of the algebra of the partially asymmetric exclusion process (PASEP) lends itself to intepretation as the transfer matrix for weighted Motzkin lattice paths and allows a succint derivation of the normalisation and correlation lengths of the PASEP from the generating function for the lattice paths. A continued fraction ("J-Fraction") representation of the lattice path generating function is particularly well suited to discussing the PASEP, for which the paths have height dependent weights.

Microcanonical analysis of polymer aggregation

Christoph Junghans
(with M. Bachmann and W. Janke)

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We propose the use of microcanonical analyses for heteropolymer aggregation transitions [1, 2]. Performing multicanonical Monte Carlo simulations of a simple hydrophobic-polar continuum model for interacting heteropolymers of finite length, we find a first-order-like behavior in the transition region between the phases of fragmented and aggregated configurations.

References

[1] C. Junghans, Diploma Thesis, Universität Leipzig (2006).

[2] C. Junghans, M. Bachmann, and W. Janke, Phys. Rev. Lett. **97** (2006) 218103.

Gradient critical phenomena in Ising quantum chain

Dragi Karevski

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We consider the behaviour of a critical system in the presence of a gradient perturbation of the couplings. In the direction of the gradient an interface region separates the ordered phase from the disordered one. We develop a scaling theory for the density profiles induced by the gradient perturbation which involves a characteristic length given by the width of the interface region. The scaling predictions are tested in the framework of the mean-field Ginzburg-Landau theory. Then we consider the Ising quantum chain in a linearly varying transverse field which corresponds to the extreme anisotropic limit of a classical two-dimensional Ising model. The quantum Hamiltonian can be diagonalized exactly in the scaling limit where the eigenvalue problem is the same as for the quantum harmonic oscillator. The energy density, the magnetization profile and the two-point correlation function are studied either analytically or by exact numerical calculations. Their scaling behaviour are in agreement with the predictions of the scaling theory [cond-mat/0611213].

Scaling theory for logarithmic-correction exponents

Ralph Kenna

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Multiplicative logarithmic corrections frequently characterize critical behaviour in statistical physics. Here it is shown that the various exponents of such corrections are interrelated just as the exponents characterizing leading scaling behaviour are. A new set of scaling relations for these logarithmic-correction exponents are proposed. These relations are then confronted with results from the literature and new predictions for logarithmic corrections in certain models are made [cond-mat/0608127].

Fun with computational physics: Non-commutative geometry on the lattice

Harald Markum[1]
(with Alberto de Campo[2]**, Wolfgang Frisch**[1]**, Harald Grosse**[3]**, and Natascha Hörmann**[1]**)**

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[2] Institute of Electronic Music and Acoustics, University for Music and Dramatic Arts, Graz, Austria
[3] Institute of Theoretical Physics, University of Vienna, Austria
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Theories with non-commutative space-time coordinates represent alternative candidates of grand unified theories. We discuss U(1) gauge theories in 2 dimensions on a lattice with N sites. Its mapping to a U(N) one-plaquette model in the sense of Eguchi and Kawai can be used for computer simulations. The choice of the boundary conditions leads to a torus or to sphere. We are interested in the confinement mechanism and in topological objects. Methods of sonification will be demonstrated in addition to graphical visualization of observables at the CompPhys06 Workshop. We are using program packages for audio browsing developed within the interdisciplinary research project SonEnvir (http://sonenvir.at/).

Fractal dimension of domain walls in two-dimensional Ising spin glasses

Oliver Melchert

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We study the problem of finding domain wall excitations on 2d Ising spin glasses in terms of a shortest path problem. Purpose of this groundstate study is to shed light on the fractal dimension d_f of domain walls, where d_f describes the scaling of the mean domain wall length with the system size L, i.e. $\bar{\ell} \propto L^{d_f}$. While our estimates for d_f in case of continuous disorder support previous findings, we are able to give a lower and an upper bound for the fractal dimension of domain walls for the case of bimodal disorder that exhibits a high degeneracy of groundstates and thus, allows for numerous domain walls with minimal energy.

Tube picture of polymers

Thomas Neuhaus

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We study polymers at finite tube thickness and with attractive interactions. The ground state of short chains exhibits only few conformational building blocks, which we attempt to classify.

Football fever: Goal distributions in football

Andreas Nußbaumer[1]
(with E. Bittner[1]**, M. Weigel**[2]**, and W. Janke**[1]**)**

[1] Institut für Theoretische Physik, Universität Leipzig, Germany
[2] Mathematics Department, School of Mathematics and Computer Sciences and the Maxwell Institute for Mathematical Sciences, Heriot-Watt University, Edinburgh, Scotland, United Kingdom
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Analyzing football score data with statistical techniques, we investigate how the highly co-operative nature of the game is reflected in averaged properties such as the distributions of scored goals for the home and away teams. It turns out that in particular the tails of the distributions are *not* well described by independent Bernoulli trials, but rather well modeled by negative binomial or generalized extreme value distributions. To understand this behavior from first principles, we suggest to modify the Bernoulli random process to include a simple component of *self-affirmation* which seems to describe the data surprisingly well and allows to interpret the observed deviation from Gaussian statistics. The phenomenological distributions used before can be understood as special cases within this framework. We analyzed historical football score data from many leagues in Europe as well as from international tournaments and found the proposed models to be applicable rather universally. In particular, here we compare men's and women's leagues and the separate German leagues during the cold war times and find some remarkable differences.

Operator product expansion on the lattice: Analytic Wilson coefficients

Holger Perlt

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We present first results for Wilson coefficients of operators up to first order in the covariant derivatives for the case of Wilson fermions. They are derived from the off-shell Compton scattering amplitude $\mathcal{W}_{\mu\nu}(a, p, q)$ of massless quarks with momentum p. The Wilson coefficients are classified according to the transformation of the corresponding operators under the hypercubic group H(4). We give selected examples for a special choice of the momentum transfer q. All Wilson coefficients are given in closed analytic form and in an expansion in powers of a up to first corrections [hep-lat/0610064].

Diffusion of the transverse magnetization profil in quantum spin chains

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The dynamic of the transverse magnetization of the Ising and XX quantum chains is studied. We use an inhomogeneous initial state obtained by setting in contact several systems, initially equilibrated at a given temperature. The relaxation behaviour is considered in the system-bath case, where a part of the chain called the system is thermalized at temperature T_s and the remaining part is at temperature T_b. In this case we derive analytically the Green function associated to the transverse magnetization in the scaling limit. For the XX model only, in the droplet situation and in the critical region $h < 1$, we show that the transverse magnetization of the system part relaxes in a finite time. This time scale diverges at the critical point $h = 1$, leading to algebraic relaxation.

Diffusion on disordered fractals

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Diffusion in disordered media shows anomalous behavior for certain length scales. In order to model anomalous diffusion random-walks on regular fractals were usually used. Here we study disordered fractals in an attempt to capture the random nature of the disordered material by randomly mixing different Sierpinski carpet generators. In particular, we investigate the diffusion on the resulting fractals by random-walk simulations and exact enumeration. We find that the random-walk exponent d_w shows a strong dependence on the mixture composition. Beyond that we consider the influence of external fields on the movement of the diffusing particles.

Simulation of shear-driven aggregation

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Aggregation of colloids has an impact on various technical as well as biological systems. Consider for example the accumulation of dust in bearings, or the clotting within blood vessels. We study a two-dimensional toy model of a colloidal suspension under shear stress. The rather novel simulation method of collision-driven dynamics has been implemented together with powerful interval arithmetics. We find two distinct fractal dimensions interpreted as cross-over from kinetic aggregation to percolation in a jamming transition. Different structural regimes of the system have been found and analyzed.

Spacetime approach to phase transitions

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The critical properties of the 3D Ising and XY models are numerically studied in the high-temperature representation. In this program, which provides an example of the spacetime approach to phase transitions, Monte Carlo simulations are performed directly on the purely geometric high-temperature graphs. With the help of percolation observables it is shown that the graphs proliferate right at the thermal critical temperature and that their fractal structure encodes the critical behavior of these models.

Architecture of randomly evolving idiotypic networks

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We investigate a minimalistic model of the idiotypic network of B-lymphocytes where idiotypes are represented by bitstrings encoding the nodes of a network. A node is occupied if a lymphocyte clone of the corresponding idiotype exists at the given moment, otherwise it is empty. There is a continuous influx of new B-lymphocytes of randomly generated idiotype from the bone marrow. B-lymphocytes are stimulated to proliferate if their receptors are cross-linked by complementary structures. Unstimulated lymphocytes die. Thus, the links of the network connect nodes encoded by complementary bitstrings allowing for a few mismatches.

The random evolution leads to a network of highly organized architecture depending on only few parameters. The nodes can be classified into different groups according to their distinct properties (e.g the mean life time). We report on the building principles, which allow to calculate analytically characteristics previously found by simulation such as the group sizes, the number of links between the groups and the mean life time.

Solution behavior of semiconductor-binding peptides

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Recent experiments have identified peptides with adhesion affinity for GaAs and Si surfaces. Here we use all-atom Monte Carlo (MC) simulations with implicit solvent to investigate the behavior in aqueous solution for four such peptides, all with 12 residues. At room temperature, we observe that all the four peptides are largely unstructured, which is consistent with experimental data. At the same time, it turns out that one of the peptides is structurally different and more flexible,

compared to the others. This finding points at structural differences as a possible explanation for varying adhesion properties of the four peptides. By also analyzing designed mutants of two of the peptides, an experimental test of this hypothesis is proposed.

Coherent destruction of the current through molecular wires using short laser pulses

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A molecular wire coupled to two electron reservoirs is investigated within a tight-binding approach including spin and Coulomb interaction. Under the assumption of weak coupling to the electron reservoirs a quantum master equation can be derived for the electron transport through the wire. Motivated by the phenomenon of coherent destruction of tunneling for monochromatic laser fields, the influence of Gaussian laser pulses on the transport through the wires is studied. For situations in which the maximum amplitude of the electric field fulfills the conditions for the destructive quantum effect the average current through the system can be suppressed. Turning on the electron correlation does not destroy the suppression of the current by the laser.

Harmonic measure probing of DLA clusters

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We develop a technique for probing harmonic measure of the diffusion limited aggregation (DLA) cluster surface with the variable size particle and generate one thousand clusters with 50 million particles using original off-lattice killing-free algorithm. Taking, in sequence, the limit of the vanishing size of the probing particles and then sending the growing cluster size to infinity, we achieve an unprecedented accuracy determining the fractal dimension, $D = 1.7100(2)$, crucial to characterization of geometric properties of the DLA clusters.

Surface segregation of conformationally asymmetric polymer blends

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We have generalized the Edwards' method of collective description of dense polymer systems in terms of effective potentials to polymer blends in the presence of a surface. With this method we have studied conformationally asymmetric athermic polymer blends in the presence of a hard wall to the first order in effective potentials, and have derived that stiffer polymers are in excess in the vicinity of the wall. For polymers with the same gyration radius R_g but different statistical segment lengths l_A and l_B the excess concentration of stiffer polymers at the surface is derived as $\delta\rho_A(z=0) \sim (l_B^{-2} - l_A^{-2})\ln(R_g^2/l_c^2)$, where l_c is a local length below of which the incompressibility of the polymer blend is violated. For polymer blends differing only in degrees of polymerization the shorter polymer enriches the wall.

Master equation and two heat reservoirs

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We analyze a simple spin-flip process under the presence of two heat reservoirs. While one flip process is triggered by a bath at temperature T, the inverse process is activated by a bath at a different temperature T'. The situation can be described by using a master equation approach in a second quantized Hamiltonian formulation. The stationary solution leads to a generalized Fermi-Dirac distribution with an effective temperature T_e. Likewise the relaxation time is given in terms of T_e. Introducing a spin-representation we perform a Landau expansion for the averaged spin $\langle\sigma\rangle$ as order parameter and consequently, a free energy functional can be derived. Owing to the two reservoirs the model is invariant with respect to a simultaneous change $\sigma \leftrightarrow -\sigma$ and $T \leftrightarrow T'$. This new symmetry generates a third order term in the free energy which gives rise a dynamically induced first-order transition [cond-mat/0608354].

System size dependence of chemical potentials and phase equilibria of bulk fluids and thin fluid films

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Using diverse particle insertion simulation methods [1,2] we study chemical potentials and fluid phase equilibria in bulk fluids and planar molecular layers. We focus on chemical potential versus density isotherms. In the subcritical temperature range we observe van der Waals-like loops in these isotherms. Applying a Maxwell equal area rule we estimate the vapour-liquid coexistence densities from the simulated isotherms [3]. Recently MacDowell *et al.* [4] reported grand canonical MC simulations of Lennard-Jones fluids and observed a distinct system size dependence of the van der Waals-like loops for subcritcal chemical potential isotherms. In this paper we study the influence of the system size on the chemical potentials of bulk square-well fluids and thin square-well films over a wide range of densities using canonical MC simulations with test particle insertions. Preliminary results show on subcritical temperatures in the density gap between the vapour and the liquid density significant finite size effects in the chemical potential while in the stable gaseous and liquid ranges the system size dependence is found to be quite weak. These findings are in qualitative agreement with the results of MacDowell *et al.* [4] On the other hand estimating the vapour-liquid coexistence properties by thermodynamic integration over the chemical potential versus density isotherms (via the equal area rule) we find only weak finite size effects on the coexistence densities and chemical potentials. A trend is observed that on fluid layers these effects are slightly larger than on bulk fluids [5].

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Collapse and freezing transitions of polymers on regular lattices

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We present simulation results for the thermodynamical behavior of flexible polymers (Interacting self-avoiding walks) on simple-cubic (sc) and face-centered cubic (fcc) lattices. Beside the well-known collapse transition, we concentrate ourselves on the freezing transition ocurring at lower temperatures.

We show how this transition, also called crystallization, liquid-solid [1] or globule-groundstate transition [2], is influenced by the lattice and how the transition depends on the system size.

We employ the pruned-enriched Rosenbluth method (PERM) [3] and generalized extensions of it [4, 5].

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Network dynamics: Laplacian of graphs and their local and global topology

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The relation between the global and local topology of a network and its Laplacian (or more specific: of a polymer and its dynamic behavior) is a fundamental question, which even for the simplest case of Rouse dynamics becomes non-trivial for general hyperbranched structures. The seminal work of Zimm and Kilb (1959) on polymers with star topology has since been extended to more general hyperbranched polymers. We present some resent mainly analytical results on this relation for regular structures such as dendrimers (finite generation Cayley trees) or hierarchically built macromolecules (fractal structures) and randomly branched polymers considering also applications of this theory to the dynamics of scale free networks. Concerning the local topology we focus on the influence of overall repeated local structures. Introducing such substructures at all places into a macromolecule that is otherwise of general topology gives rise to a characteristic change of the Laplacian spectrum of the relaxation modes. We show that for specific such substructures the eigen-frequencies of the extended and the reduced structures are related by polynomial equations that can be determined by a real-space renormalization step. The global topologies that we study, are characterized by either a regular hierarchy, which can again be treated by real-space renormalization or, if they are random, by the possibility of forming large possibly percolating structures. In combination of both approaches the latter may be decorated by additional local structures.

Networks interacting with matter

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Dynamics on complex networks have attracted a great attention recently. Many systems can be studied with the assumption that the timescale for processes taking place on networks is different from the evolution of connections between nodes. In this short talk I would like to present a simple model where these two timescales are of the same order as a result of an interaction between the matter and the geometry.

Frustration from fat graphs

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A zoo of random graphs and surfaces has attracted the attention of physicists in recent decades: generic and scale free (small-world) random graphs, "thin" or mean-field type random graphs, Voronoï-Delaunay triangulations, and the "fat" random graphs of the dynamical triangulations approach to quantum gravity — to name only a few. Apart from studying the generic geometrical and topological properties of these graphs, interest has focused on the effect of placing matter variables such as the spin models of statistical mechanics on these structures to see whether changes in universal behavior can be observed. Apart from certain attempts to use random graphs as computational tools for the mean-field theory of spin glasses, most studies have considered the situation of plain (Ising, Potts, ...) ferromagnets, where the effect of random connectivity is rather mild in that an ordered phase persists and only the character of the phase transition changes. Here, instead, we consider what happens for the case of *antiferromagnets*, where geometrical disorder interferes with the requirement of bipartiteness crucial for the existence of the Néel state. Some general speculations (and pointers to the literature) concerning the behavior of such systems on "thin" and "fat" random graphs are followed by an investigation of the Ising antiferromagnet on quenched, fat ϕ^3 graphs using exact ground-state computations. We find a zero-temperature spin-glass phase equivalent to that of the bimodal Ising spin glass on the same geometry.

Percolation of vortex networks in the U(1) lattice Higgs model

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We study the properties of vortex networks in the $U(1)$ lattice Higgs model in $d = 3$ dimensions. Specifically we investigate the percolation behaviour of those networks at a point in the parameter space of the theory where we see a crossover from confining to non-confining behaviour in observables, which is not accompanied by a thermodynamic phase transition. Recently, we argued that this crossover

can be regarded as a Kertèsz line [1]. The present study wants to explicitly determine the critical behaviour of those clusters. To get independent and unbiased results for critical exponents we have developed an automated tool in conjunction with multihistogramm reweighting which maximises the data collapse quality. For the clusters under consideration here, we get exponents that are compatible with ordinary percolation theory. However, the cluster percolation threshold does not strictly coincide with the crossover point from local thermodynamic observables (energy) in the non-first order regime. This is a problem also observed in different contexts [2].

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Rare-event sampling in local sequence alignments

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Sequence alignment is a tool in molecular biology to detect similarity in protein sequences (or DNA). A measure of the similarity is the optimal alignment score of a pair of sequences. Under a random sequence model the score can be interpreted as a random variable. Its distribution is a relevant quantity in significance assessment of protein database queries. In the case of infinitely long sequences and gapless alignments the score follows a Gumbel distribution. Less is known about the case of finite sequences and gapped alignments, where empirical studies give evidence that the Gumbel form is still valid in the high probability range of the distribution. Here we present a method to obtain the distribution on a wide range, including the rare event tail down to $p \sim 10^{-40}$. This problem is similar to the problem of obtaining the density of states of a complex physical system and therefore methods from statistical mechanics could be adopted: By parallel tempering, the tail was accessed and the distribution could be obtained over a wide support by histogram reweighting. We present the results for different scoring schemes, in detail: pairwise optimal alignment, sum of k-best alignments, position dependent alignment each with different score matrices and gap costs. In most cases we find Gaussian deviations from Gumbel in the tail of the distribution, which is not accessible with naive sampling schemes. Since significance assessment rely on the tail of the distribution, such deviations should not be neglected in practice. Furthermore we find qualitatively differences between standard alignment and position dependent alignment, which is used in searching transmembrane proteins.

Surface diffusion in potential landscapes

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We study 2D surface diffusion with different types of potential landscapes. As test potentials we use Gaussian and power-law distributions with or without correlations. For these model surfaces we investigate diffusion properties that will be the basis to understand the inverse problem: Getting potential lanscapes from surface diffusion measurements. For this purpose, we try to determine a possible basis of potentials and their diffusion properties for a direct transformation from the experimental results to the underlying potential within the pore.

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