ABSTRACTS

of contributions to the

8th International NTZ-Workshop on
New Developments in Computational Physics

CompPhys07

Institut für Theoretische Physik,
Universität Leipzig, Germany

29 Nov – 01 Dec 2007

`http://www.physik.uni-leipzig.de/~janke/CompPhys07`

Supported by the Centre for Theoretical Sciences (NTZ) of the Centre for Advanced Study (ZHS) of Universität Leipzig, 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 Deutsch-Französische Hochschule, the PPP Collaborative Research Programme of the DAAD, and the Deutsche Forschungsgemeinschaft.

Abstracts

Modelling nanotubes and their applications with atomistic simulations

Joan Adler

Technion, Haifa, 32000 Israel

phr76ja@tx.technion.ac.il

Carbon nanotubes have a wide variety of actual and potential applications, and are small enough that modeling of these applications on a atomistic scale is possible, if not easy. Two diverse applications under study at the Technion are nanotubes as separators of diffusing molecules (physics/chemical engineering) and nanotubes as mass sensors in NEMS (physics/electrical engineering). Both projects use Molecular Dynamics: in the former this is combined with Grand Canonical Monte Carlo in dual control volumes. We model the nanotube atoms with a Reactive Empirical Bond Potential, and use predictor-corrector variants for the equations of motion in the diffusion project and Verlet in the mass-sensor one. In the former the nature of the diffusion and of the molecular separation is studied for different loadings and molecular mixtures and in the latter the thermal vibrations are calculated. In both cases great attention to the "statistical mechanical" aspects such as equilibration are required. In the former an exploration of diffusion behaviour in rigid versus flexible nantubes was made. In the latter initial results in agreement with an analytic calculation of a special case were found. Vizualization and animation with our Atomistic Visualization package AViz of the dynamics has been carried out for both debugging and presentation purposes and these can be viewed at http://phycomp.technion.ac.il/~phr76ja/leipzig.

Folding of proteins using Monte Carlo simulations

Pedro Armando Ojeda May
Universität Kassel, Germany
pojeda@physik.uni-kassel.de

We present simulations of the folding process using the energy landscape method and reweighted histogram simulations. We calculate the thermodynamical properties of the peptide V3-loop of the VIH virus with 16 amino acids. Simulations under spatial confinement of proteins is also studied.

Adsorption of multi-block and random copolymers on a solid surface

Swati Bhattacharya
Max Planck Institute for Polymer Research, Mainz, Germany
bhattach@mpip-mainz.mpg.de

The adsorption of a single multi-block AB-copolymer on a solid planar substrate is investigated by means of computer simulations and scaling analysis. It is shown that the problem can be mapped onto an effective homopolymer adsorption problem. In particular we discuss how the critical adsorption energy and the fraction of adsorbed monomers depend on the block length M of sticking monomers A, and on the total length N of the polymer chains. Also the adsorption of the random copolymers is considered and found to be well described within the framework of the annealed approximation. For a better test of our theoretical prediction, two different Monte Carlo (MC) simulation methods were employed: a) off-lattice dynamic bead-spring model, based on the standard Metropolis algorithm (MA), and b) coarse-grained lattice model using the Pruned-enriched Rosenbluth method (PERM) which enables tests for very long chains. The findings of both methods are fully consistent and in good agreement with theoretical predictions.

Replica-exchange cluster algorithm

Elmar Bittner and Wolfhard Janke

Institut für Theoretische Physik, Universität Leipzig, Germany
elmar.bittner@itp.uni-leipzig.de

In typical finite-size scaling analyses of Monte Carlo simulations of a model exhibiting a second-order phase transition, one often needs an extended temperature/energy range around the critical point. By combining the replica-exchange algorithm with cluster updates and an adaptive routine to find the range of interest, we introduce a new flexible and powerful method for systematic investigations of second-order phase transitions. As a result, we gain two further orders of magnitude for 2D and 3D Ising models in comparison with the recently proposed Wang-Landau recursion for cluster algorithms based on the multibondic algorithm, which is already a great improvement over the standard multicanonical variant.

Multifractal properties of self-avoiding walks on percolation clusters

Viktoriya Blavatska

Institut für Theoretische Physik, Universität Leipzig, Germany
blavatska@itp.uni-leipzig.de

The model of self-avoiding walks (SAWs) on disordered lattice perfectly describes the universal properties of long flexible polymer chains in porous media. In our study, disordered lattice is exactly at the percolation threshold. Applying the pruned-enrichment Rosenbluth chain-growth method (PERM), we perform numerical simulations of SAWs on the backbone of the incipient percolation cluster in two, three and four dimensions. Considering higher-order correlations of SAWs, we study the multifractal properties of the model. Our results bring about the estimates of critical exponents, governing the scaling laws of configurational properties of SAWs.

On the phase structure of 3D Abelian two-Higgs model on the lattice

Martin Bock

IZMB Bonn, Germany

bock@itp.uni-leipzig.de

We investigate non-perturbative features of a three-dimensional Abelian Higgs model with singly- and doubly-charged scalar fields coupled to a single compact Abelian gauge field. The model is pretending to describe various planar systems of strongly correlated electrons. The behavior of three kinds of topological defects – holon and spinon vortices and monopoles – is explored in various phases. We also observe a new effect, the strong enhancement of the phase transition strength reflected in a lower order of the transition at certain model parameters.

Phase separation of two-component systems in thin films

Katarzyna Bucior

(with Leonid Yelash and Kurt Binder)

Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany

bucior@uni-mainz.de

We use a coarse-grained model of hexadecane dissolved in supercritical carbon dioxide to simulate the phase separation, initiated by quenching a system into an unstable region of the phase diagram, e.g. by temperature or pressure jumps. The parameters of the model are fitted to reproduce critical parameters of hexadecane and carbon dioxide. The study is performed in slit like pores, formed by two infinite parallel walls consisting of spherical particles. We present the typical results for the observed time evolutions during phase separation for this model, structure factors, snapshot pictures, density profiles, density distributions. Since the behavior of the system depends on the distance from the wall, we calculate some properties in layers parallel to the walls. The time dependence of the characteristic domain size is also discussed.

Free zero-range process on networks

Zdzisław Burda

Institute of Physics and Mark Kac Complex Systems Research Centre, Jagellonian University, Krakow, Poland

burda@th.if.uj.edu.pl

We discuss a stochastic process which describes a gas of particles hopping between neighboring sites of the given network with the hopping rate depending only on the occupation of the departure site. The process has a steady state with a condensate of particles on a single network site. We compare static and dynamical properties of the condensate on homogeneous and heterogeneous networks.

Anomalously localized electronic states in three-dimensional disordered samples

Philipp Cain

(with Michael Schreiber)

Institute of Physics, Chemnitz University of Technology, Germany

cain@physik.tu-chemnitz.de, schreiber@physik.tu-chemnitz.de

We study the Anderson model of localization at the metal-insulator transition in the band centre of three-dimensional disordered samples. For the critical disorder we determine a large number of wave functions of the model and study the distribution of the wave function amplitudes. Deviations from scaling of multifractal correlation functions allow us to discriminate anomalously localized states from the usual critical states. The thus identified anomalously localized states lead to deviations of the critical properties and should be eliminated from the ensemble average for a characterization of criticality.

Thermodynamics of a protein model with warm and cold denaturations

Olivier Collet

LPM, Nancy-Université, CNRS, Boulevard des Aiguillettes BP239, F-54506 Vandoeuvre-lès-Nancy, France

olivier.collet@lpm.u-nancy.fr

A four states phase diagram for protein folding as a function of temperature and solvent quality is derived from an improved 2-d lattice model taking into account the temperature dependence of the hydrophobic effect. The phase diagram exhibits native, globule and two coil-type regions. In agreement with experiment, the model reproduces the phase transitions indicative of both warm and cold denaturations. Finally, it predicts transitions between the two coil states and a critical point.

Adaptive simulation resolution: basic principles and applications

Luigi Delle Site

Max-Planck Institute for Polymer Research Mainz, Germany

dellsite@mpip-mainz.mpg.de

For the study of complex synthetic and biological molecular systems by computer simulations one is still restricted to simple model systems or to by far too small time scales. To overcome this problem multiscale techniques are being developed for many applications. However in almost all cases, the regions of different resolution are fixed and not in a true equilibrium with each other. We here give the theoretical framework for an efficient and flexible coupling of the different regimes. The approach leads to an analog of a geometry induced phase transition and a counterpart of the equipartition theorem for fractional degrees of freedom. This provides a rather general formal basis for advanced computer simulation methods applying different levels of resolution.

Accurate prediction of protein structures – how to find the exact ground state

Frank Dressel[1,2]

(with Sigismund Kobe[1] **and M. Schroeder**[2]**)**

[1] Institut für Theoretische Physik, TU Dresden, Germany
[2] Biotechnologisches Zentrum, TU Dresden, 01062 Dresden, Germany
frank.dressel@biotec.tu-dresden.de

Since the emergence of the famous Levinthal paradoxon [1] and its proposed solution by Bryngelson et al. [2] it is one of the open questions, whether or not the native state is really the ground state of the interacting amino acid system in proteins. We extended a coarse grained model [3] by including sequence similarity. Within its context we are able to reproduce the native state with high accuracy. For many proteins (up to 70 amino acids) we performed exact optimization and found in most cases the ground state in good agreement with the native state.

[1] C. Levinthal, in: Mossbauer Spectroscopy in Biological Systems: Proceedings of a meeting held at Allerton House, ed. by J.T.P. De-Brunner and E. Munck (University of Illinois Press, Monticello Illinois 1969), pp. 22–24.
[2] J.D. Bryngelson, J.N. Onuchic, N.D. Socci, and P.G. Wolynes, Proteins: Structure, Function, and Genetics 21, 167 (1995).
[3] F. Dressel and S. Kobe, Chem. Phys. Lett. 424, 369 (2006).

Entanglement evolution after connecting finite to infinite quantum chains

Viktor Eisler

FU Berlin, Germany
eisler@physik.fu-berlin.de

We consider quantum chains which are initially separated and in their ground states. After connecting them the quantum state evolves and the entanglement increases. It is found that the entanglement entropy displays a typical behaviour which is common for the different geometries considered. It is characterized by a rapid rise to values larger than in equilibrium followed by a slow relaxation. For critical systems the lattice results are in a very good agreement with predictions of conformal field theory.

Long-range correlated random field and random anisotropy O(N) models

Andrei Fedorenko
LPT ENS Paris, France
andrei.fedorenko@lpt.ens.fr

We study the long distance behavior of the O(N) model in the presence of random fields and random anisotropies correlated as $\propto 1/x^{d-\sigma}$ for large separation x using the functional renormalization group. We compute the fixed points and analyze their regions of stability within a double $\epsilon = d-4$ and σ expansion. We find that the long-range disorder correlator remains analytic but generates short-range disorder whose correlator develops the usual cusp. This allows us to obtain the phase diagrams in (d, σ, N) parameter space and compute the critical exponents to first order in ϵ and σ. We show that the standard renormalization group methods with a finite number of couplings used in previous studies of systems with long-range correlated random fields fail to capture all critical properties.

Solution-space structure of (some) optimization problems

Alexander Hartmann
Institute for Physics, University of Oldenburg, Germany
a.hartmann@uni-oldenburg.de

We study numerically the cluster structure of random ensembles of two NP-hard optimization problems originating in computational complexity, the vertex-cover problem and the number partitioning problem. We use branch-and-bound type algorithms to obtain exact solutions of these problems for moderate system sizes. Using two methods, direct neighborhood-based clustering and hierarchical clustering, we investigate the structure of the solution space. The main result is that the correspondence between solution structure and the phase diagrams of the problems is not unique. Namely, for vertex cover we observe a drastic change of the solution space from large single clusters to multiple nested levels of clusters. In contrast, for the number-partitioning problem, the phase space looks always very simple, similar to a random distribution of the lowest-energy configurations. This holds in the "easy"/solvable phase as well as in the "hard"/unsolvable phase.

The critical behavior of 3D Ising glass models: universality and scaling corrections

Martin Hasenbusch

Dipartimento di Fisica, Universita di Pisa, Italy, and Institut für Theoretische Physik, Universität Leipzig, Germany

hasenbus@ifh.de, martin.hasenbusch@itp.uni-leipzig.de

We perform high-statistics Monte Carlo simulations of three three-dimensional Ising spin-glass models: the $\pm J$ Ising model for two values of the disorder parameter p, $p = 1/2$ and $p = 0.7$, and the bond-diluted $\pm J$ model for bond-occupation probability $p_b = 0.45$. A finite-size scaling analysis of the quartic cumulants at the critical point shows conclusively that these models belong to the same universality class and allows us to estimate the scaling-correction exponent ω related to the leading irrelevant operator, $\omega = 1.0(1)$. We also determine the critical exponents ν and η. Taking into account the scaling corrections, we obtain $\nu = 2.53(8)$ and $\eta = -0.384(9)$.

Phase-ordering kinetics in disordered two-dimensional Ising models

Malte Henkel

Laboratoire de Physique des Materiaux, Université Nancy I, France

henkel@lpm.u-nancy.fr

The phase-ordering kinetics of the ferromagnetic two-dimensional Ising model with uniform disorder is investigated by intensive Monte Carlo simulations. Taking into account finite-time corrections to scaling, simple ageing behaviour is observed in the two-time responses and correlators. The dynamical exponent z and the form of the scaling functions only depend on the ratio ϵ/T, where ϵ describes the width of the distribution of the disorder. The agreement of the predictions of local scale-invariance generalised to $z \neq 2$ for the two-time scaling functions of response and correlations with the numerical data provides a direct test of generalised Galilei-invariance.

Anisotropic Heisenberg antiferromagnets in two dimensions

Martin Holtschneider[1], Walter Selke[1], Stefan Wessel[2], and R. Leidl[1]

[1] Institut für Theoretische Physik, RWTH Aachen, Germany
[2] Institut für Theoretische Physik III, Universität Stittgart, Germany
selke@physik.rwth-achen.de

Square lattice Heisenberg antiferromagnets with uniaxial anisotropy in a field along the easy axis have been studied [1,2,3]. Based on ground state considerations and Monte Carlo simulations, the role of biconical structures in the transition region between the antiferromagnetic nd spin–flop phases is analysed. In particular, adding a single-ion anisotropy to the XXZ antiferromagnet, one observes, depending on the sign of that anisotropy, an intervening biconical phase or a direct transition of first order separating the two phases. In case of the anisotropic XY model, the degeneracy of the ground state, at a critical field, in antiferromagnetic, spin-flop, and bidirectional structures seems to result, as in the case of the XXZ model, in a narrow disordered phase, with bidirectional fluctuations, in between the antiferromagnetic and spin–flop phases.

[1] M. Holtschneider, W. Selke, and R. Leidl, Phys. Rev. B 72, 064443 (2005).
[2] M. Holtschneider, S. Wessel, and W. Selke, Phys. Rev. B 75, 224417 (2007).
[3] M. Holtschneider and W. Selke, Phys. Rev. B (Rapid Comm., in print) [cond-mat/0710.1251].

Escape transition of grafted polymer chains from a cylindrical tube

Hsiao-Ping Hsu

Institut für Physik, Johannes Gutenberg-Universität, Mainz, Germany
hsu@uni-mainz.de

A grafted polymer chain confined in a finite cylindrical tube of length L and diameter D undergoes an abrupt transition when the number of monomers in the chain, N, reaches a critical value. This problem has the merit that it is potentially very relevant for experiments and application such as the problem of polymer translocation through pores in membranes. In order to check the theoretical prediction based on the Landau free energy approach, similar as our previous work in $2d$ [1], we study $3d$ single polymer chains with excluded volume interactions and with one end grafted

at the inner wall of a cylindrical tube, by simulating self-avoiding walks on a simple cubic lattice with finite cylindrical confinement. A biased sequential sampling algorithm with re-sampling, similar to the pruned-enriched Rosenbluth method (PERM) [2,3] is used. The difficulty of obtaining correct samplings for the first-order phase transition is solved by pulling the free chain end with different strength of force out from the tube, and reweighting the biased configuration. We estimate the free energy, the end-to-end distance, the number of imprisoned monomers, the order parameter, and its distribution. It is shown that in the thermodynamic limit of large N and L but finite L/N, there is a very pronounced jump in several average characteristics, including the order parameter. All simulation results are in good agreement with the analytical theory.

[1] H.-P. Hsu, K. Binder, L. I. Klushin, and A. M. Skvortsov, Phys. Rev. E **76**, 021108 (2007).
[2] P. Grassberger, Phys. Rev. E **56**, 3682 (1997).
[3] H.-P. Hsu and P. Grassberger, Eur. Phys. J. B **36**, 209 (2003).

Entanglement of quantum many-body systems

Ferenc Iglói

Research Institute for Solid State Physics and Optics, Budapest, Hungary
igloi@szfki.hu

The entanglement entropy of the two-dimensional random transverse Ising model is studied with a numerical implementation of the strong disorder renormalization group. The asymptotic behavior of the entropy per surface area diverges at, and only at, the quantum phase transition that is governed by an infinite randomness fixed point. Here we identify a double-logarithmic multiplicative correction to the area law for the entanglement entropy. This contrasts with the pure area law valid at the infinite randomness fixed point in the diluted transverse Ising model in higher dimensions.

Lattice paths and the PASEP

Desmond A. Johnston

Math. Dept., Heriot-Watt University, Edinburgh, EH14 4AS, UK
des@ma.hw.ac.uk

The matrix representation of the algebra of the partially asymmetric exclusion pro-

cess (PASEP) lends itself to intepretation as the transfer matrix for weighted 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 representation of the lattice path generating function is particularly well suited to discussing the PASEP, for which the paths have height dependent weights. We use this as our principal tool in extracting the phase behaviour.

Controlling material properties using a thermostat

Christoph Junghans

Max-Planck-Institut für Polymerforschung (MPI-P), Mainz, Germany
junghans@mpip-mainz.mpg.de

An extension to the dissipative particle dynamics thermostat is studied, which on the one side keeps the stabilizing and hydrodynamic properties, but on the other side allows to control the dynamical properties of the system. Treating the friction or the transversal and longitudinal components of the relative velocities of interacting pairs separately enables to adjust diffusion constant and shear viscosity to the desired value. Analytical predictions are confirmed by numerical simulations of a repulsive Lennard-Jones fluid. A very sensitive dependency of the viscosity and diffusion constant on the strength of the friction is observed.

Tensor decomposition in electronic structure calculations on 3D Cartesian grids

Venera Khoromskaia

Max Planck Institute for Mathematics in the Sciences, Leipzig, Germany
vekh@mis.mpg.de

In this paper we propose a novel approach based on the combination of Tucker-type and canonical tensor decomposition techniques for the efficient numerical approximation of functions and operators in electronic structure calculations. In particular, we study potential applications of tensor approximations for the numerical solution of Hartree-Fock and Kohn-Sham equations on 3D Cartesian grids. Low-rank orthogonal Tucker-type tensor approximations are investigated for electron densities and Hartree potentials of simple molecules, where exponential convergence with respect to the Tucker rank is observed. This enables an efficient tensor-product convolu-

tion scheme for the computation of the Hartree potential using a collocation-type approximation via piecewise constant basis functions on a uniform grid. Our approach exhibits fast convergence, and for large 3D grids (of size $n \times n \times n$), our tensor-product convolution scheme with complexity $O(n)$ markedly outperforms the traditional 3D-FFT in both the computing time and storage requirements.

Lattice-Boltzmann simulations of particle suspensions in a sheared flow

Eric Lorenz

University of Amsterdam, The Netherlands
elorenz@science.uva.nl

We report two-dimensional particle simulations using the Lattice-Boltzmann method. In the limit of small solid-fraction ϕ and Reynolds number Re suspension rheolgy is well understood and described by analytical or semiempirical functions. We performed direct simulations for dense suspensions up to relatively high Re where hydrodynamical interaction between solid and fluid and particle-particle interaction are the governing momentum-exchange processes and lead to an increased viscosity η in a shear flow, known as shear-thickening. To measure η for pure bulk suspension we developed an extension of Lees-Edwards boundary conditions for LBM to particle suspensions. We therefore are able to overcome the problem of wall artefacts in suspension rheology observed in commonly used Couette flow schemes. Furthermore we investigated characteristics and size distribution of particle clusters as clustering is believed to be the significant process leading to shear thickening.

Percolation of negative-weighted loops on 2d lattices

Oliver Melchert

Institut für Physik, Universität Oldenburg, 26111 Oldenburg, Germany
melchert@theorie.physik.uni-oldenburg.de

We describe a percolation problem on 2d lattice-graphs, with edge weights drawn from disorder distributions that allow for weights of either sign. Minimal-weighted configurations of negative-weighted loops are obtained and system spanning loops are observed above a certain fraction of negative edge weights. Exploring square lattices with side-length up to $L = 512$, we numerically determine the critical exponents

that describe this geometric transition. The results are found to be close to the random-bond Ising model at $T = 0$. Further, we address the question of universality by investigating different types of the bond disorder.

Aggregation and mechanical unfolding of proteins

Simon Mitternacht

Computational biology and biological physics group, Department of Theoretical Physics, Lund University, Sweden

simon@thep.lu.se

Using all-atom Monte Carlo (MC) simulations with implicit water combined with a cluster size analysis, we study the aggregation of Ab(16-22), a peptide capable of forming amyloid fibrils. We consider a system of six peptides, and investigate the thermodynamics and structural properties of aggregates formed by this system. The system is unaggregated at high temperature, and forms beta-sheet rich aggregates at low temperature. At the crossover between these two regimes, we find that clusters of all sizes occur, whereas the beta-strand content is low. We also observe the spontaneous formation of a beta-barrel with six antiparallel strands. The beta-barrel stands out as the by far most long-lived aggregate seen in our simulations. Single-molecule experiments on a fibronectin type III domain show that this protein unfolds via intermediates when stretched by an external force. Simulation and mutation studies have suggested that there is more than one intermediate, but it was not possible to determine which intermediate is seen in a specific event. To elucidate the unfolding pathway of this protein, we performed unfolding simulations both with a constant force, and a constant pulling-velocity. Using the Jarzynski relation we measure the free energy as a function of end-to-end distance and are thus able to estimate the unfolding free energy difference as function of force and the equilibrium unfolding force.

Evaporation/condensation of Ising droplets

Andreas Nußbaumer, Elmar Bittner, and Wolfhard Janke

Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany

andreas.nussbaumer@itp.uni-leipzig.de

In [1] Biskup *et al.* study the behaviour of finite-volume liquid-vapour systems at a fixed excess N of particles above the ambient gas density. They identify a di-

mensionless parameter Δ and a universal constant Δ_c 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 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 condensed phase, at various system sizes ($L = 40, \ldots, 640$). Using analytic values for the spontaneous magnetisation m_0, the susceptibility χ and the free energy τ_W of a droplet with Wulff shape for the infinite system, we were able to determine λ in very good agreement with the theoretical prediction [2]. The measurements were repeated on a triangular lattice and for the next-nearest neighbour interaction, giving similarly good results.

[1] M. Biskup, L. Chayes, and R. Kotecky, Europhys. Lett. 60, 21 (2002).
[2] A. Nußbaumer, E. Bittner, T. Neuhaus, and W. Janke, Europhys. Lett. 75, 716 (2006).

Perturbative determination of c_{SW} with Symanzik improved gauge action and stout smearing

Holger Perlt

Institut für Theoretische Physik, Universität Leipzig, Germany
holger.perlt@itp.uni-leipzig.de

We determine the improvement factor c_{SW} in one-loop lattice perturbation theory for the plaquette and Symanzik improved gauge actions. The fermionic action is $\mathcal{O}(a)$ clover improved with one-time stout smearing. c_{SW} is derived from the one-loop correction to the quark-quark-gluon vertex in the off-shell regime. We give a first numerical value for the one-loop contribution to the non gauge-invariant improvement coefficient c_{NGI} for the quark field using the plaquette action. A discussion of mean-field improvement is included.

A precision simulation of SU(3) gauge theory in 2+1 dimensions and the continuum limit

Bengt Petersson

Fakultät für Physik, Universität Bielefeld, Germany
bengt@physik.hu-berlin.de

We have performed a precision calculation of SU(3) lattice gauge theory at finite temperature in $2+1$ dimensions. We take the continuum limit. In particular the phase transition and the thermodynamics in the deconfined state are discussed. We also discuss lessons for simulations at finite temperature in $3+1$ dimensions.

Work fluctuations in small quantum spin chains

Thierry Platini

Laboratoire de Physique des Matériaux, Université Henri Poincaré, Nancy I, France
platini@lpm.u-nancy.fr

We study the work fluctuations of two types of finite quantum spin chains under the application of a time-dependent magnetic field in the context of the fluctuation relation and Jarzynski equality. For several magnetic field protocols, the quantum Crooks and Jarzynski relations are numerically tested and fulfilled. As a more interesting situation, we consider the forcing regime where a periodic magnetic field is applied. For a non-integrable chain, we show that depending on the field frequency a sharp transition is observed between a Poisson limit work distribution at high frequencies toward a normal work distribution at low frequencies.

Adaptive resolution simulation of liquid water

Matej Praprotnik

Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128 Mainz, Germany
praprot@mpip-mainz.mpg.de

We present a multiscale simulation of liquid water where a spatially adaptive molecular resolution procedure allows for changing on-the-fly from a coarse-grained to an

all-atom representation. We show that this approach leads to the correct description of all essential thermodynamic and structural properties of liquid water.

Fractal dimensions of loop gases on fluctuating lattices

Adriaan Schakel

Institut für Theoretische Physik, Freie Universität Berlin, Germany
schakel@physik.fu-berlin.de

Loop gases on fluctuating random planar lattices are discussed both in the dilute limit and at the point where the loops collapse, known as the theta point in polymer physics. Starting from the known fractal dimensions on regular planar lattices, we use the Knizhnik-Polyakov-Zamolodchikov formula of quantum gravity to predict the fractal dimensions of such loop gases coupled to gravity. A comparison with Monte Carlo simulations of the Potts model on random lattices is given.

The lattice gluon propagator in numerical stochastic perturbation theory

Arwed Schiller

Institut für Theoretische Physik, Universität Leipzig, Germany
arwed.schiller@itp.uni-leipzig.de

We calculate loop contributions up to four loops to the Landau gauge gluon propagator in numerical stochastic perturbation theory. For different lattice volumes we carefully extrapolate the Euler time step to zero for the Langevin dynamics derived from the Wilson action. The one-loop result for the gluon propagator is compared to the infinite-volume limit of standard lattice perturbation theory.

Randomly evolving idiotypic networks: a mean-field approach

Holger Schmidtchen and Ulrich Behn

Institut für Theoretische Physik and IMPRS Mathematics in the Sciences,
Universität Leipzig, POB 100 920, 04009 Leipzig, Germany
holger.schmidtchen@itp.uni-leipzig.de, ulrich.behn@itp.uni-leipzig.de

B-Lymphocytes express on their surface receptors (antibodies) of a given specifity (idiotype). Crosslinking these receptors by complementary structures, antigens or antibodies, stimulates the lymphocyte. Thus a large functional network of interacting lymphocytes, the idiotypic network, emerges. Idiotypic networks conceived by Niels Jerne 30 years ago, experience a renewed interest [1], e.g. in the context of autoimmune diseases. In a previously proposed minimalistic model [2] idiotypes are represented by bitstrings. The population dynamics of the idiotype clones is reduced to a zero-one scheme. An idiotype survives only if it meets enough but not too much complementary structures. We investigate the random evolution of the network towards a highly organized functional architecture which is driven by the influx of new idiotypes, randomly generated in the bone marrow. The nodes can be classified into different groups, which are clearly distinguished by their statistical characteristics. They include densely connected core groups and peripheral groups of isolated nodes, resembling central and peripheral part of the biological network. We found the building principles of the observed architecture which allows to calculate analytically size and linking of the groups [3]. In a mean-field approach mean occupation of the groups and mean life time of occupied nodes are determined and compared with simulation results.

[1] U. Behn, Idiotypic networks: toward a renaissance?, Immunol. Rev. 216, 142-152 (2007).

[2] M. Brede and U. Behn, Patterns in randomly evolving networks: Idiotypic networks, Phys. Rev. E 67, 031920 (2003).

[3] H. Schmidtchen and U. Behn, Randomly evolving idiotypic networks: analysis of building principles, in: Artificial Immune Systems, H. Bersini and J. Carneiro (Eds.), Lecture Notes in Computational Sciences 4163, Springer-Verlag, Berlin Heidelberg (2006), pp. 81–94.

The critical Binder cumulant – revisited

Walter Selke[1] **and Lev N. Shchur**[2]

[1] Institut für Theoretische Physik, RWTH Aachen, Germany
[2] Landau Institute, Chernogolovka, Russia
selke@physik.rwth-achen.de

The critical Binder cumulant for the two-dimensional Ising model with nearest and asymmetric next-nearest neighbour interactions on a square lattice and with nearest neighbour interactions on a triangular lattice has been studied using Monter Carlo techniques [1,2,3]. In particular, the role of the boundary condition, of the shape of the system, and of the anisotropy of the critical correlations are discussed and compared to renormalization group arguments by Dohm and Chen (see the following references).

[1] W. Selke and L.N. Shchur, J. Phys. A 38, L739 (2005).
[2] W. Selke, Eur. Phys. J. B 51, 223 (2006).
[3] W. Selke, J. Stat. Mech., P04008 (2007).

Critical amplitude ratios of 3-state and 4-state Potts model

Lev N. Shchur

(with Bertrand Berche and Paolo Butera)

Landau Institute for Theoretical Physics, Chernogolovka, Moscow region, Russia
lev@landau.ac.ru

Monte Carlo (MC) simulations and series expansions (SE) data for the energy, specific heat, magnetization and susceptibility of the 3-state and 4-state Potts model on the square lattice are analyzed in the vicinity of the critical point to estimate universal combinations of critical amplitudes. Estimation of the critical amplitudes needs knowledge of the correction-to-scaling exponents. We use those predicted by conformal field theory. We construct effective ratios of quantities close to the critical point and analyze how they approach critical amplitude ratios. In particular, we found that for the Potts model with any number of states q the effective ratio of energy amplitudes approach unity always linearly.

Our results for the amplitude ratios of 3-state Potts model definitely agree with the theoretical predictions and earlier numerical estimates for the specific-heat and the susceptibility amplitude ratios.

We improve quality of the fits for the 4-state Potts model using prediction of renormalization group (RG) to fit data in the appropriate temperature window. We explore RG prediction on the cancelation of logarithmic corrections in the universal amplitude ratio. The ratios of the susceptibility critical amplitudes of 4-state Potts model obtained in our analysis differ from those predicted theoretically and supported by earlier SE and MC analyzes.

The collapse dynamics of a classical Brownian self-gravitating system: analogy with the chemotactic aggregation and with the Bose-Einstein condensation

Julien Sopik

Jacobs University Bremen, Germany
j.sopik@jacobs-university.de

In this talk, I will introduce the collapse dynamics of a classical Brownian self-gravitating system. I will show that this dynamics can also describe the chemotactic aggregation dynamics of biological populations. This dynamics exhibits also striking similarities with the Bose-Einstein condensation of a gas of free bosons strongly coupled with a thermal bath.

Skeleton expansions for directed polymers in disordered media

Semjon Stepanow

Institut für Physik, Universität Halle, 06099 Halle, Germany
semjon.stepanow@physik.uni-halle.de

Partial summations of perturbation expansions of the directed polymer in disordered media (DPRM) enables one to represent the latter as skeleton expansions in powers of the effective coupling constant $\Delta(t)$, which corresponds to the binding state between two replicas in the replica field theory of DPRM, and is equivalent to the binding state of a quantum particle in an external δ-potential. The strong coupling phase is characterized by the exponential dependence of $\Delta(t)$ on t, $\Delta(t) \sim \exp(p_c t)$ with p_c being the binding energy of the particle. For dimensions $d > 2$ the strong coupling phase exists for $\Delta_0 > \Delta_c(d)$. We compute explicitly the mean-square displacement

and the 2nd cumulant of the free energy to the lowest order in powers of effective coupling in $d = 1$. We argue that the elimination of the terms $\exp(p_c t)$ in skeleton expansions demands an additional partial summation of skeleton series.

How to overcome free energy barriers in grandcanonical Monte Carlo simulations

Peter Virnau

Institut für Physik, Universität Mainz, Germany
virnau@uni-mainz.de

Grandcanonical Monte Carlo simulations are currently the method of choice when it comes to determining phase diagrams. At low temperatures, however, free-energy barriers arise and need to be overcome. In this talk, I will discuss several strategies, including a rather novel algorithm called Successive Umbrella Sampling. I will also present some recent applications – the phase diagram of a coarse-grained model for CO_2 and the phase diagram of a simple colloid-polymer mixture model.

Freezing and collapse of flexible polymers

Thomas Vogel

(with Michael Bachmann and Wolfhard Janke)

Institut für Theoretische Physik, Universität Leipzig, Germany
thomas.vogel@itp.uni-leipzig.de

We analyze the crystallization and collapse transition of a simple model for flexible polymer chains on simple cubic and face-centered cubic lattices by means of sophisticated chain-growth methods. In contrast to bond-fluctuation polymer models in certain parameter ranges, where these two conformational transitions were found to merge in the thermodynamic limit, we conclude from our results that the two transitions remain well-separated in the limit of infinite chain lengths. The reason for this qualitatively distinct behavior is presumably due to the ultrashort attractive interaction range in the lattice models considered here.

Polymer stars and DNA in correlated environments

Christian von Ferber

Applied Mathematics Research Centre, Coventry University, UK
c.vonferber@coventry.ac.uk

While weak uncorrelated disorder has long been shown not to influence the scaling properties of polymers in solution, we find significant effects of disorder that is long-range correlated. A partly surprising result is that the impact on the configurational entropy of star branched polymers is opposite to the corresponding impact on linear chains. We discuss consequences for mixtures of linear and star branched polymers and for the denaturation transition of DNA in a correlated environment.

Multicanonical simulations of complex networks

Bartłomiej Wacław[1]

(with Leszek Bogacz[2] **and Wolfhard Janke**[1]**)**

[1] Institut für Theoretische Physik, Universität Leipzig, Germany
[2] Department of Information Technologies, Jagellonian University, Krakow, Poland
waclaw@itp.uni-leipzig.de

The science of complex networks, studied extensively over the last decade, became an important part of statistical physics. A variety of methods has been used to explain structural properties of networks and the influence of their topology on some processes on them. Some of the proposed models can only be studied by means of computer simulations and many algorithms have been invented to generate different networks. In this short talk we would like to present an extension of a method developed earlier by us. The method relies on sampling of a statistical ensemble of networks by means of a Monte Carlo algorithm, performing local updates in the graph structure. Since the same idea has been frequently used in simulations of spin systems like the Ising model, it is not surprising that methods like multicanonical simulations can be borrowed and applied also to networks. We will show this for the example of the degree distribution, where by increasing the probability of occurrence of high-degree nodes one is able to study finite-size effects with a much larger precision than in normal simulations.

Aging in fully-frustrated spin systems

Jean-Charles Walter

Laboratoire de Physique des Matériaux, Université Henri Poincaré, Nancy I, France
walter@lpm.u-nancy.fr

We study the aging properties of the fully-frustrated clock model (FFCM) with two and three states (these models are equivalent to the fully-frustrated Ising model (FFIM) and the fully-frustrated three-state Potts model (FFPM)). A model is said to be fully-frustrated when each plaquette is frustrated. This is the case on a square lattice when each plaquette contains three ferromagnetic (resp. antiferromagnetic) bonds and one anti-ferromagnetic (resp. ferromagnetic) bond. We restricted ourselves to such a coupling configuration called Zig-Zag.

The FFIM has been solved exactly by Villain [1]. The phase diagram of the FFPM has been studied numerically by Foster et al. [2]. Both models display a paramagnetic phase at non-vanishing temperature and undergo a phase transition to the ferromagnetic phase at zero temperature. We study these two models by means of Monte Carlo simulations with Glauber dynamics on a square lattice (lattice size 192×192 and periodic boundary conditions). The system is initially prepared in the paramagnetic phase and then quenched at the critical temperature. In a such a situation, homogeneous ferromagnets display aging due to the competition between the different ordered phases [3]. We study the large-time behaviour of the spin-spin autocorrelation functions, the response to a magnetic field and the fluctuation-dissipation ratio. We observed the existence of aging. We give estimates of the exponents λ/z and $a_c = 2\beta/\nu z$ and of the asymptotic value $X_{\rm inf}$ of the fluctuation-dissipation ratio. These quantites are believed to be universal [4]. The FFIM has logarithmic corrections. The FFPM seems to follow the same behaviour although the data are not so conclusive.

[1] J. Villain, J. Phys. C 10, 1717 (1977).
[2] D. P. Foster, C. Gerard, and I. Puha (2001), J. Phys. A 34, 5183 (2001).
[3] A. J. Bray, Adv. Phys. 43, 357 (1994).
[4] C. Godrèche and J. M. Luck, J. Phys. A 33, 9141 (2000).

Optimization through extra dimensions: the Ising spin glass

Martin Weigel

Institut für Physik, KOMET 331, Johannes Gutenberg-Universität Mainz, Germany
weigel@uni-mainz.de

Quite generally, metastability disappears as the dimension of the underlying phase space is made sufficiently large as the system acquires additional possibilities to escape from a local minimum using the extra dimensions. Here, this observation is used to solve the ground-state problem of Ising spins by mapping it into an interacting particle system in a high-dimensional space and evolving it in a molecular dynamics simulation.

On the phase structure of 3D Abelian one-Higgs model on the lattice

Sandro Wenzel

Institut für Theoretische Physik, Universität Leipzig, Germany
sandro.wenzel@itp.uni-leipzig.de

We study the properties of vortex networks in the $U(1)$ lattice Higgs model in $d = 3$ dimensions. Specifically, we investigate network percolation properties at a point in the parameter space of the theory where we see a distinct crossover from confining to non-confining behaviour in local 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 aim of the present study is to explicitly determine the scaling behaviour of those global clusters and to give direct evidence of our previous argument. 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 scaling exponents that are compatible with ordinary percolation theory.

[1] S. Wenzel, E. Bittner, W. Janke, A.M.J. Schakel, and A. Schiller, Phys. Rev. Lett. **95**, 051601 (2005).

Author Index