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ABSTRACTS

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New Developments in Computational Physics

CompPhys11

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Preface

As in previous years, also the 12th International NTZ-Workshop *CompPhys11* on *New Developments in Computational Physics* covers a broad spectrum of different fields ranging from general aspects of computational and statistical physics over applications in condensed and soft matter physics, including biological applications, and random networks to the intriguing properties of quantum systems and high-energy physics. And following the tradition, also this year's Workshop is designed to provide a forum for an informal exchange of ideas and to meet in a relaxed atmosphere in Leipzig at the beginning of Christmas time.

The Workshop takes place from 24 – 26 November 2011 in the Lecture Halls ("Kleiner Hörsaal" and "Theorie Hörsaal") and the "Aula" of the Experimental Physics building. We are very grateful to all colleagues who helped moving their regular lecture courses to another place or date, and in particular to Dr. Konrad Schiele who successfully coordinated this difficult task. We also wish to thank the secretaries of the Institute for Theoretical Physics, Ms. Susan Hussack, Ms. Gabriele Menge, and Ms. Lea Voigt, for their invaluable help with all administrative matters.

Finally, we and the Centre for Theoretical Sciences (NTZ) gratefully acknowledge financial support of the Workshop from Research Academy Leipzig (RALeipzig), Top Level Research Area PbF2 (Mathematical Sciences), DFG Research Group 877, DFG SFB/TRR 102, Deutsch-Französische Hochschule (DFH-UFA), Alexander von Humboldt Foundation, and DFG Graduate School of Excellence "BuildMoNa".

Leipzig, November 2011
Wolfhard Janke

Abstracts

Finite-dimensional Edwards-Anderson spin glass: Evidence of phase transition at nonzero magnetic field

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We present results from parallel tempering Monte Carlo simulations of a four-dimensional bimodal Edwards-Anderson (EA) spin glass with binary couplings in the presence of an external magnetic field. The correlation functions display a strongly non-Gaussian behavior. We must, therefore, introduce a somewhat non standard finite-size scaling analysis. We find clear evidence of a phase transition for finite values of the magnetic field. Furthermore, we are able to determine the set of critical exponents over the Almeida-Thouless line. These exponents clearly differ from those at zero magnetic field.

Numerical simulations of Faraday waves in binary Bose-Einstein condensates

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We show by extensive numerical simulations and analytical variational calculations that binary non-miscible Bose-Einstein condensates subject to periodic modulations of the radial confinement exhibit a Faraday instability similar to that seen in one-component condensates. Considering the $|1,-1\rangle$ and $|2,-2\rangle$ hyperfine states of realistic ^{87}Rb condensates, we show that there are two experimentally relevant stationary state configurations: The one in which the components form a dark-bright symbiotic pair (the ground state of the system), and the one in which the components are segregated (first excited state). For each of these two configurations, we show numerically that far from resonances the Faraday waves excited in the two components are of similar periods, emerge simultaneously, and do not impact the dynamics of the bulk of the condensate. Finally, we show that for a modulation frequency close to twice that of the radial trapping, the emergent surface waves fade out in favor of a forceful collective mode that turns the two condensate components miscible.

Gaussian universality class of mixed quantum spin chains (P)

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We simulate two different mixed-spin quantum Heisenberg models and find critical lines with continuously varying critical exponents. The sine-Gordon model, a Gaussian model with an irrelevant perturbation, is known to exhibit the same phenomenon. The critical properties of the Gaussian model are fully specified by two continuously varying parameters, the fundamental scaling dimension and the characteristic velocity. We extract several critical exponents of the mixed quantum spin chains. If they belong to the Gaussian universality class, all exponents should be expressible by a single fundamental scaling dimension. As we find good yet not conclusive agreement with this prediction we put forward further evidence for the Gaussian nature of mixed quantum chains from direct calculation of the Gaussian parameters and the central charge.

Parallel-tempering cluster algorithm for computer simulations of critical phenomena

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In finite-size scaling analyses of Monte Carlo simulations of second-order phase transitions one often needs an extended temperature range around the critical point. By combining the parallel tempering algorithm with cluster updates and an adaptive routine to find the temperature window of interest, we introduce a flexible and powerful method for systematic investigations of critical phenomena [1]. As a result, we gain one to two orders of magnitude in the performance 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.

[1] E. Bittner and W. Janke, Phys. Rev. E **84** (2011) 036701.

Polymer adsorption on a fractal substrate

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We study the adsorption of flexible polymer macromolecules on a percolation cluster, formed by a regular two-dimensional disordered lattice at critical concentration p_c of attractive sites. The percolation cluster is characterized by a fractal dimension $d_s^{p_c} = 91/49$. The conformational properties of polymer chains grafted to such a fractal substrate are studied by means of the pruned-enriched Rosenbluth method (PERM). We find estimates for the surface crossover exponent governing the scaling of the adsorption energy in the vicinity of the transition point, $\phi_s^{p_c} = 0.425 \pm 0.009$, and for the adsorption transition temperature, $T_A^{p_c} = 2.64 \pm 0.02$. As expected, the adsorption is diminished when the fractal dimension of the substrate is smaller than that of a plain Euclidean surface. The universal size and shape characteristics of a typical spatial conformation which attains a polymer chain in the adsorbed state are analyzed as well. In particular, for the averaged asphericity the value $\overline{\langle A_2^{p_c} \rangle} = 0.483 \pm 0.006$ is obtained, indicating a higher isotropy of adsorbed conformations compared with the case of a plain attractive surface.

TRAVIS – A free analyzer and visualizer for MC and MD trajectories (P)

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We present TRAVIS ("TRajectory Analyzer and VISualizer"), a free program package for analyzing and visualizing Monte Carlo and molecular dynamics trajectories. The aim of TRAVIS is to collect as many analyses as possible in one program, creating a powerful tool and making it unnecessary to use many different programs for evaluating simulations. This should greatly rationalize and simplify the workflow of analyzing trajectories. TRAVIS is written in C++, open-source freeware and licensed under the terms of the GNU General Public License (GPLv3). It is easy to install (platform independent, no external libraries) and easy to use. On this poster, we present some of the algorithms that are implemented in TRAVIS – many of them widely known for a long time, but some of them also to appear in literature for the first time. All shown analyses only require a standard MD trajectory as input data.

Scale-free enumeration of self-avoiding walks on critical percolation clusters (P)

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We present a new method for exact enumeration of self-avoiding walks on critical percolation clusters. It can handle very long walks by exploiting the clusters' low connectivity and self-similarity. In 2D we were able to enumerate walks of more than 1000 steps with over 10^{170} conformations.

Hierarchic genetic strategy for solving inverse problems (P)

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The main idea of the research is an application of the Hierarchic Genetic Strategy (HGS) in inverse problems. HGS performs efficient concurrent search in the optimization landscape by many small populations. We present hp-HGS genetic strategy (hp-adaptive Finite Element Method combined with HGS) for solving parametric inverse problems. The efficiency of the proposed strategy results from coupling an adaptive accuracy of solving optimization problems with the accuracy of hp-FEM problems. As a case study we use a deformation problem in Step-and-Flash Imprint Lithography, a modern patterning process utilizing photopolymerization to replicate the topography of a template onto a substrate. The considered problem is more sensitive to one of the parameters. In order to overcome this difficulty, as well as to narrow down the search space, we use a hierarchical approach in stages.

Importance of single nodes for Boolean network dynamics

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Boolean networks are time- and state-discrete dynamical systems with applications in modeling gene-regulatory processes, among others. With the help of such models, the importance of each single node (gene, protein) can be quantified as the probability that perturbing the node's initial state alters the long-term dynamics. The scenario resembles the analysis of damage spreading in spin kinetics. Measuring node importance has potential implications for identifying key players, e.g., elements that determine the development of undifferentiated cells into a specific cell type. We provide analytical and numerical evidence that the eigenvector centrality, i.e., the leading eigenvector of the adjacency matrix, yields a good proxy of node importance. Accuracy is improved further when the analysis is based on a weighted adjacency matrix with the weights (so-called activities) quantifying the dependence of Boolean functions on their inputs. Both randomly generated systems and regulatory networks of real biological systems are analyzed.

Complex temperature zeros in the partition function of the 3D Ising model

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Complex temperature zeros of the partition function represent an alternative approach to obtain information about critical behavior. Both the location of the zeros and their impact angle with the real axis provide information about critical exponents and universal amplitudes ratios. In this work we use a high-precision Monte Carlo simulation to determine the universal specific-heat amplitude ratio A_+/A_- in the three-dimensional Ising model. We also measure the correlation-length critical exponent ν from finite-size scaling and the specific-heat exponent α through hyperscaling. Using this uncommon approach, we obtain results compatible with some previous accurate estimates from a variety of sources and rule out recently conjectured exact values.

[1] A. Gordillo-Guerrero, R. Kenna, and J.J. Ruiz-Lorenzo, *Universal amplitude ratios in the Ising model in three dimensions*, e-print arXiv:1107.1186.

Random-field Ising magnet with correlated disorder

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We study the correlated-disorder driven zero-temperature equilibrium phase transition of the random-field Ising magnet (RFIM) using exact numerical ground-state calculations for cubic lattices. We consider correlations of the quenched disorder decaying proportional to r^a, where r is the distance between two lattice sites and $a < 0$. To obtain exact ground states, we use a well established mapping to the graph-theoretical maximum-flow problem, which allows us to study large system sizes of more than two million spins. We use finite-size scaling analyses for values $a = \{-1, -2, -2.5, -3, -7\}$ to calculate the critical point and the critical exponents characterizing the behavior of the specific heat, magnetization, susceptibility and of the correlation length close to the critical point. We find basically the same critical behavior as for the RFIM with delta-correlated disorder, except for the finite-size exponent of the susceptibility and for the case $a \geq -2$, where the results are also compatible with a phase transition at infinitesimal disorder strength. We numerically confirm earlier predictions. A summary of this work can be found at the papercore database www.papercore.org.

A Monte Carlo study of surface critical phenomena: The special point

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We study the special point in the phase diagram of a semi-infinite system where the bulk transition is in the three-dimensional Ising universality class. To this end we performed a finite-size scaling study of the improved Blume-Capel model on the simple cubic lattice with two different types of surface interaction. In order to check for the effect of leading bulk corrections we also simulated the spin-1/2 Ising model on the simple cubic lattice. We accurately estimated the surface enhancement coupling at the special point of these models. We find $y_t = 0.718(2)$ and $y_h = 1.6465(6)$ for the surface renormalization group exponents of the special transition [1]. These results are compared with previous ones obtained by using field-theoretic methods and Monte Carlo simulations of the spin-1/2 Ising model. Furthermore, we study the behavior of the surface transition near the special point, and finally we discuss films with special boundary conditions at one surface and fixed ones at the other.

[1] M. Hasenbusch, Phys. Rev. B **84** (2011) 134405.

Oscillations in delayed SIRS model on homogeneous networks (P)

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We studied delayed SIRS model on a random homogeneous network and compared the result with mean-field solution of delayed and standard SIRS. In delayed SIRS for some intervals of variables we can observe oscillation. We studied these oscillations and showed that mean field properly fits random homogeneous network. So we used the mean-field solution as an equivalent for the network. Then we focused on two diminutional lattice model as a lattice case of homogeneous network with $z = 4$. We studied spatio-temporal behavior of the lattice and saw infection waves in the lattice.

Logarithmic extensions of local scale invariance

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Systems such as two-dimensional critical percolation are known to be described by a so-called logarithmic extension of conformal invariance, which involves to associate logarithmic partners with the scaling operators of the theory. Here, we shall consider an analogous extension of local scale invariance, which is conceived to describe among others ageing phenomena far from equilibrium. Application to growth phenomena, described by the 1D Kardar-Parisi-Zhang equation, and as well to critical 1D directed percolation will be discussed.

Structure and scaling analysis of stretched semiflexible polymer chains

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Semiflexible polymer chains under good solvent conditions are described by self-avoiding walks on the square and simple cubic lattices in $d = 2$ and $d = 3$ dimensions, respectively, and the stiffness of chains is controlled by the bending energy ϵ_b. In our previous work [1, 2] with the pruned-enriched Rosenbluth methed (PERM), we have observed a double crossover behavior, rigid-rod-like to (almost) Gaussian random coils, then to self-avoiding walks, for the chain length up to $N = 50\,000$ in $d = 3$, but only a single crossover from rigid-rod-like to self-avoiding walks for the chain length up to $N = 25\,600$ in $d = 2$. Testing the applicability of the Kratky-Porod model, we have also checked whether the chain conformation is dominated by the excluded volume effects or not as the chain length and its flexibility vary. However, the extension versus force curve is still not well understood if the stretching force is applied to one end of polymer chains although a plenty of literature exists. We therefore extend our study to the problem of stretching semiflexible chains. Varying the strength of the force, the flexibility of the chain, and the chain length, the theoretical predictions of the force-extension relationship at different length scale regimes (linear response – Pincus blob – Kratky-Porod model – freely jointed chain) are checked. Our large-scale Monte Carlo simulations give clear evidence for the importance of excluded volume effects on the stretching behavior of semiflexible polymer chains [3].

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[2] H.-P. Hsu, W. Paul, and K. Binder, Europhys. Lett. **95** (2011) 68004.
[3] H.-P. Hsu and K. Binder, e-print arXiv:1110.1410.

Quantum relaxation after a quench in systems with boundaries

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We study the time-dependence of the magnetization profile, $m_l(t)$, of a large finite open quantum Ising chain after a quench [1]. We observe a cyclic variation, in which starting with an exponentially decreasing period the local magnetization arrives to a quasi-stationary regime, which is followed by an exponentially fast reconstruction period. The non-thermal behavior observed at near-surface sites turns over to thermal behavior for bulk sites. Besides the standard time and length scales a non-standard time scale is identified in the reconstruction period.

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Gonihedric Ising models: Order parameter(s) and dual(s)

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The family of 3D Gonihedric Ising models defined by Savvidy and Wegner display a planar flip symmetry intermediate between a global and a gauge symmetry and as a consequence do not possess a standard magnetic order parameter. An anisotropic variant of the purely plaquette version of this model, originally discussed as the "Fuki-Nuke" model by Suzuki, is non-trivially equivalent to a stack of 2D Ising models, each of which can magnetize independently at the phase transition point. Consideration of the anisotropic model suggests that a suitable order parameter in the isotropic case should be a form of planar magnetization. We conduct simulations to investigate this and related candidate order parameters in the isotropic plaquette Gonihedric model and its dual.

The two-dimensional Ising spin glass at zero temperature (P)

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Ground states for the Ising spin glass in two dimensions can be determined in polynomial time as long as periodic boundary conditions are applied at most in one direction. Using a recently proposed mapping to an auxiliary graph decorated with Kasteleyn cities, we determine ground states for systems with open-periodic boundary conditions for lattices of linear sizes up to $L = 9000$ and calculate defect energies as well as domain-wall lengths. Although the matching approach does not work for periodic-periodic boundaries, where less finite-size corrections are expected, using a windowing technique allows to determine quasi-exact ground-states for lattices up to $L = 3000$. By using these techniques, we arrive at high-precision estimates of the spin-stiffness exponent and the domain-wall fractal dimension for Gaussian as well as bimodal couplings. We compare the geometry of the thus generated domain walls with the detailed predictions given for random curves in the plane in the framework of Schramm-Loewner Evolution (SLE).

Mythological networks

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As in statistical physics, notions of universality exist within the field of comparative mythology. However there is no quantitative classification system to facilitate comparison of myths. Here, network theory is applied to a variety of mythologies to quantify their characteristics. In this way, myths can be compared across different cultures and to other networks, both actual and fictitious in an effort to discover where they are positioned along the spectrum from the real to the imaginary.

Mean-field behavior of the negative-weight percolation model on random regular graphs

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In a previous study, carried out on regular lattice graphs in dimensions $d = 2$ through 7, it was suggested that the negative-weight percolation (NWP) problem has an upper critical dimension $d_u = 6$ [1]. Here, we investigate the critical properties of minimum-weight loops and paths in the NWP problem on 3-regular random graphs (RRGs), i.e., graphs where each node has exactly 3 neighbors and were there is no regular lattice structure. By studying a particular model on RRGs, one has direct access to the mean-field exponents that govern the model for $d > d_u$. In this regard, the presented study aims to support the previous conjecture $d_u = 6$ by directly computing the mean-field exponents for the NWP model with a bimodal weight distribution, and comparing them to those found for a regular hypercubic lattice with dimension $d = 6$. The presented results are obtained via computer simulations as well as by analytic means. The numerical simulations are based on a mapping to an appropriate minimum-weight perfect matching problem for which fast algorithms exist, and the analytic approach utilizes a correspondence between the NWP problem and the problem of polymers in random media which is then studied by means of the replica symmetric cavity method. We find that the numerical values for the critical exponents on RRGs, as well as those obtained using the replica symmetric cavity method for the related polymer problem, agree with those found for $d = 6$-dimensional hypercubic lattice graphs within error bars and hence support the conjectured upper critical dimension $d_u = 6$ [2].

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Optimization by local heat pulse – quenching cycles by means of GULP

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We present an optimization algorithm for problems with a large number of continuous degrees of freedom which often exhibit extremely many local minima. It is based on the thermal cycling approach which had originally been developed for combinatorial optimization tasks [1]. The basic idea of our approach is to cyclically disturb a few degrees of freedom of the current best local minimum and to quench this state by a highly efficient local search code. In this, the amplitude of the disturbance slowly decreases. This approach is applied to a lattice structure prediction problem. Thus we use the general utility lattice program (GULP) by J.D. Gale and co-workers [2] as local search code. As a test case, the energy landscape of the $Mg_{10}Al_4Ge_2Si_8O_{36}$ lattice is investigated, where the interactions are modelled by Buckimham and three-body potentials [3], and where the cell parameters are free to vary. In the talk, we compare various versions of our approach differing with respect to the choice of the modified degrees of freedom. The results testify that the procedure is robust and far more efficient than the

previous approaches to the same test problem by means of simulated annealing and multi-start local search in Ref. [3]. Moreover, it can be easily parallelized.

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Comparison of grafted and non-grafted polymer adsorption in different ensembles (P)

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In the present work, we compare the thermodynamic behavior of a finite single free polymer near an attractive substrate with that of a polymer grafted to that substrate. After we recently found first-order like signatures in the microcanonical entropy at the adsorption transition in the free case [2], and knowing that many studies on the polymer adsorption in the past have been performed for grafted polymers, the question arises, to what extent and in what way the grafting changes the natures of the adsorption transition. This question is tackled here using a coarse-grained off-lattice model and covers not only the adsorption transition, but all transitions a single polymer near an attractive substrate of varying strengths undergoes. Due to the impact of grafting especially on the translational but also on the conformational entropy of desorbed chains, the adsorption transition is affected the strongest. Our results are obtained by a combined canonical and microcanonical analysis of Monte Carlo data.

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Confined systems: New theory and applications

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Adsorption of fluids in mesopores is often accompanied by the phenomenon of hysteresis, i.e., the amount adsorbed from the gas phase is not only controlled by the actual gas pressure, but may depend on the history. This is in distinct disagreement to the basic concept of thermodynamic states which are conceived to be dependent only on the actual boundary conditions. Some authors explain the existence of the adsorption hysteresis by the involvement of metastable states [1, 2]. Neimark and Visnyakov [3] discuss the construction of a ground state that incorporates the microstates of both branches of the hysteresis loop. Admittedly, this concept leads to the definition of a ground state that can never be visited experimentally. From a large number of simulations one can show that there exists a gap between the extent of validity of standard thermodynamics and observations. We claim that we have made progress in filling this gap [4]: (1) We replace the EOS by curves of states (COS); (2) A system may support more than one COS; (3) Coexistence states do not exist; (4) The system moves reversibly within a COS. It jumps from one COS to another COS only, if the experimental boundary condition cannot be fulfilled otherwise. A jump is an irreversible process. Moreover, we can show that these rules widely determine even the dynamic behavior of confined systems.

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Application of two-dimensional simulated tempering (ST) to the two-dimensional Ising model (P)

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We performed two-dimensional simulated tempering (ST) simulations of the two-dimensional Ising model in different sizes in order to investigate the phase transitions and to study the crossover behavior. In this two-dimensional ST, not only temperature but also the external field become dynamical variables updated by the Metropolis criteria. Thus, this method can be referred to as "Simulated Tempering and Magnetizing (STM)". We also performed the "Simulated Magnetizing (SM)" simulations, in which the external field was considered as a dynamic variable but temperature was not. It is shown that while ST and SM simulations cannot go over first-order phase transition lines, STM can by making a two-dimensional random walk in temperature and external field. The STM allows one to draw a phase diagram for a wide range of temperature and external field from a single simulation run. We also studied the crossover behavior of phase transitions with respect to temperature and external field.

Precision calculation of spin-spin correlators in the Ising model via worm updates

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We determine the spin-spin correlation function in the 2D Ising model via Worm updates numerically and compare the form of the correlator with the analytic prediction of Wu and McCoy.

Pair-factorised steady state model exhibits a condensate's growth on monolayers

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In this work in progress, we consider stochastic rules of mass transport which lead to steady states that factorize over the links of a one-dimensional ring. Based on the knowledge of the steady states, one can derive the onset of a phase transition from a liquid to a condensed phase that is characterized by the existence of a condensate. Previous results in 1D are broadened to approximate the model with statistical weights corresponding to Lennard-Jones potential of an adsorbent's surface. We find that the model exhibits a condensate's growth on particle monolayers, whose thickness depends on the Lennard-Jones parameter σ. We also extend the study to the condensate's shape in a 2D square lattice.

Generalized-ensemble simulations of spin models and biomolecular systems

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Conventional simulations are greatly hampered by the multiple-minima problem, where the simulations tend to get trapped in some of a huge number of local minimum energy states. In order to overcome this difficulty, we have been advocating the uses of generalized-ensemble algorithms which are based on non-Boltzmann weight factors. With these algorithms we can explore a wide range of the configurational space. The advantage of

generalized-ensemble algorithms such as the multicanonical algorithm and the replica-exchange method lies in the fact that from only one simulation run, one can obtain various thermodynamic quantities as functions of temperature. In this presentation, I will give newly developed generalized-ensemble algorithms and the latest results of various applications of generalized-ensemble simulations to spin models and biomolecular systems.

Improvement of Monte Carlo estimates with covariance-optimized finite-size scaling at fixed phenomenological coupling

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In the finite-size scaling analysis of Monte Carlo data, instead of computing the observables at fixed Hamiltonian parameters, one may choose to keep a renormalization-group invariant quantity, also called phenomenological coupling, fixed at a given value. Within this scheme of finite-size scaling, we exploit the statistical covariance between the observables in a Monte Carlo simulation in order to reduce the statistical errors of the quantities involved in the computation of the critical exponents [1]. This method is general and does not require additional computational time. This approach is demonstrated for the Ising model in two and three dimensions, where large gain factors in CPU time are obtained.

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Anisotropy impact in the 3D Heisenberg spin-glass model

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We have performed a finite-size scaling study of the three-dimensional Heisenberg spin glass in the presence of a weak random anisotropy, for lattices of size up to $L = 32$ [1]. Anisotropies play a major role in the phase transition and cause that the CG susceptibility no longer diverges at T_{CG}, the chiral glass (CG) transition temperature. It follows that the anisotropic system belongs to a universality class different from the isotropic model, which questions the applicability of the chirality scenario.

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The non-perturbative part of Wilson loops

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The non-perturbative part of Wilson loops are supposed to be related strongly to the gluon condensate – a quantity which could contribute to hadronic masses. One possible successful framework for its computation is lattice gauge theory. We present our new results for Wilson loops of various sizes in pure SU(3) gauge theory.

Strong roughening of spontaneous imbibition fronts

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Imbibition is the displacement of one fluid by another immiscible fluid in a porous matrix. The dynamics and morphological evolution of the invasion front can be described by simple scaling laws. In systems with similar

pore length and diameter such as paper and sand, the menisci advancement is highly correlated due to surface tension resulting in slow imbibition front roughening. Sponteneous imbibition experiments with a sponge like glass, in which nanopores have much longer lengths than diameters, display an anomalously fast imbibition front roughening dynamics. Guided by the microscopic structure of vycor glass we formulate a pore network model in which we study spontaneous imbibition with extensive computer simulations. Using finite-size scaling we find that the menisci in the individual capillaries propagate nearly independently, resulting in a roughening exponent close to 1/2. These results reveal a new universality class of imbibition behaviour which is expected to occur in any matrix with elongated pores.

How the maximum step size in Monte Carlo simulations should be adjusted

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Since the work by Miller, Amon, and Reinhardt, which correctly warned against the indiscriminate adjustment of the maximum step size during Monte Carlo (MC) simulations, some researchers have believed that adjusting the maximum step size always leads to systematic errors. I will demonstrate that when periodic adjustments to Monte Carlo parameters are done properly, they can improve the overall accuracy of simulations without introducing errors.

Partition function zeros and phase transitions of a polymer chain

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The zeros of the canonical partition functions for flexible square-well polymer chains have been computed for chains up to length 256 for a range of square-well diameters. We have previously shown that such chain molecules can undergo a coil-globule and globule-crystal transition as well as a direct coil-crystal transition [1]. Here we show that each of these transitions has a well-defined signature in the complex-plane map of the partition function zeros. The freezing transitions are characterized by nearly circular rings of uniformly spaced roots, indicative of a discontinuous transition. The collapse transition is signaled by the coalescence of roots onto an elliptical horse-shoe segment pinching down towards the positive real axis. For sufficiently small square-well diameter the elliptical collapse ring merges with the circular freezing ring yielding the direct coil-crystal transition. The root density of all rings increases with increasing chain length and the leading roots move towards the positive real axis, implying a divergence of the specific heat in the thermodynamic limit (as originally proposed by Yang and Lee).

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Resonance and pattern formation in the Kuramoto model with Manhattan delay

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The Kuramoto model has been succesful in explaining common synchronization phenomena such as clapping audiences, flashing fireflies or arrays of Josephson junctions. Here we present results for the Kuramoto model with the original all-to-all coupling, but we add a time delay with distance calculated on a virtual lattice according to the Manhattan (taxi-driver's) metric. The resulting system has interesting behavior in the desynchronized regime. Periodicity in the resonance frequency has been observed. Stabilized phase patterns such as plane waves and vortices have also been recorded. This is, to our knowledge, the first case of a Kuramoto model with distance-dependent delay which does not explicitly include short-ranged interactions and still produces phase patterns.

Motifs emerge from function in model gene regulatory networks

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Gene regulatory networks allow the control of gene expression patterns in living cells. The study of network topology has revealed that certain subgraphs of interactions or "motifs" appear at anomalously high frequencies. We ask here whether this phenomenon may emerge because of the functions carried out by these networks. Given a framework for describing regulatory interactions and dynamics, we consider in the space of all regulatory networks those that have prescribed functional capabilities. Markov Chain Monte Carlo sampling is then used to determine how these functional networks lead to specific motif statistics in the interactions. In the case where the regulatory networks are constrained to exhibit multistability, we find a high frequency of gene pairs that are mutually inhibitory and self-activating. In contrast, networks constrained to have periodic gene expression patterns (mimicking for instance the cell cycle) have a high frequency of bifan-like motifs involving four genes with at least one activating and one inhibitory interaction.

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