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ABSTRACTS

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New Developments in Computational Physics

CompPhys10

Institut für Theoretische Physik, Universität Leipzig, Germany

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Preface

As in previous years, also the 11th NTZ-Workshop *CompPhys10* 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 25 – 27 November 2010 in the Theory Lecture Hall ("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.

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Leipzig, November 2010
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Abstracts

Fast converging path integrals for time-dependent potentials

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We calculate the short-time expansion of the propagator for a general quantum system with many degrees of freedom in a time-dependent potential to orders that have not been accessible before. To this end the propagator is expressed in terms of a discretized effective potential, for which we derive and analytically solve a set of efficient recursion relations. Such a discretized effective potential can be used to substantially speed up numerical Monte Carlo simulations for path integrals, or to set up various analytic approximation techniques to study dynamic properties of quantum systems in time-dependent potentials. The analytically derived results are numerically verified by treating several simple models in both imaginary and real time.

[1] A. Balaz, I. Vidanovic, A. Bogojevic, and A. Pelster, *Fast converging path integrals for time-dependent potentials*, preprint arXiv:0912.2743.

The infinite-component spin glass revisited

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Replica field theory calculations describing the Sherrington-Kirkpatrick mean-field spin-glass model break down at the upper critical dimension in the course of an expansion towards finite (spatial) dimensions. In order to shed some new light on natural spin-glass models like the Heisenberg or XY model in low dimensions we bypass replica field theory and consider the replica symmetric m-component vector spin glass in the limit of large m, for which the free-energy landscape is simplified considerably. This simplification comes about through the fact that in the limit of a large number of spin components the ground state of a finite system occupies only a finite-dimensional subspace in spin space, giving rise to the concept of a generalized Bose-Einstein condensation, where spins condense into one unique state at low temperature. As a consequence, for each system size there exists a finite, critical number m^* of spin components above which the ground-state energy does not change upon further adding spin dimensions, such that the system effectively describes a spherical spin glass. Apart from the interest in the model itself, the $m = \infty$ limit might serve as a starting point for expansions towards finite m. We investigated the stability of the ordered phase numerically as a function of the spatial dimension of the lattice $d = 2, 3, \ldots$ with the $(T = 0)$ defect energy approach for extracting the stiffness exponents. Additionally, at finite temperatures, we used the spin-spin correlation function in order to cross-check results. Both approaches have been considered for both hypercubic lattices as well as the power-law one-dimensional spin glass, possessing a continuously tunable effective lattice dimension. Aim of the investigations is to determine the lower critical dimension for the m-component vector spin glass in the limit $m \to \infty$. The results are compared to estimates resulting from field-theoretic calculations.

Molecular simulation of hot nano particles (P)

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Brownian motion is a subject of continuing interest in theoretical as well experimental fields of various branches of quantitative science primarily because of its prominent role in the "middle world" between macro and micro

cosmos [1, 2]. It has become a "drosophila" for formulating and testing theories in equilibrium and nonequilibrium statistical mechanics. In this project we investigate a nonequilibrium generalization of Brownian motion, namely "Shot Brownian motion", that has so far received little attention, as a potential candidate for single molecule tracking. In our scenario, the Brownian particle is kept at an elevated temperature with respect to the surrounding fluid which is experimentally realized when a light absorbing tracer particle diffuses in the focus of a laser. Due to the separation of time scale between heat propagation and the diffusion of the nano particle a steady state temperature profile is developed around the nano particle which is easily detected by a second laser. This provides the basis for promising dynamic photo-thermal single particle tracking and correlation spectroscopy with high potential of complementing the conventional fluorescence techniques [3-6]. A recent analytical approach using fluctuating hydrodynamics and microscopic energy-entropy balance has successfully described the system in terms of effective Markovian parameters [7]. We use molecular dynamics simulations on Graphics Processing Units to investigate the various microscopic phenomena as well as microscopic/hydrodynamic boundary conditions associated with "Shot Brownian motion" which are neither directly accessible to the theory nor to experiment. These simulations are used to test the validity of the effective Markovian model and the effect of microscopic details on the continuum predictions of the theory.

[1] M. Haw, *Middle World: The Restless Heart of Matter and Life* (Macmillan, New York, 2006).
[2] E. Frey and K. Kroy, *Brownian motion: A paradigm of soft matter and biological physics*, Ann. Phys. (Leipzig) **14** (2005) 20–50.
[3] S. Berciaud, L. Cognet, G. A. Blab, and B. Lounis, Phys. Rev. Lett. **93** (2004) 2574021–4.
[4] V. Octeau *et al.*, ACS nano **3** (2009) 345.
[5] P. Paulo *et al.*, J. Phys. Chem. C **113** (2009) 11451.
[6] R. Radünz, D. Rings, K. Kroy, and F. Cichos, *Hot Brownian particles and photothermal correlation spectroscopy*, J. Phys. Chem. A **113** (2009) 1674–1677.
[7] D. Rings, R. Schachoff, M. Selmke, F. Cichos, and K. Kroy, *Hot Brownian motion*, Phys. Rev. Lett. **105** (2010) 090604-1–4.

Coupled order parameter systems on scale-free networks

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We analyse a system of two scalar order parameters on a complex scale-free network in the spirit of Landau theory. To add a microscopic background to the phenomenological approach we also study a particular spin Hamiltonian that leads to coupled scalar order behavior using the mean-field approximation. This set up may describe a model of opinion formation where, e.g., opinions on a party and a candidate are coupled. Our results show that the system is characterised by either of two types of ordering: either one of the two order parameters is zero or both are non-zero but have the same value. While the critical exponents do not differ from those of a model with a single order parameter on a scale-free network there are notable differences for the amplitude ratios and susceptibilities. Another peculiarity of the model is that the transverse susceptibility is divergent at all $T < T_c$ when $O(n)$ symmetry is present. This behavior is related to the appearance of Goldstone modes [1]. More recently we have also analysed the logarithmic corrections found at marginal values of the exponent that governs the scale-free degree distribution of the network. We derive and verify scaling relations between them [2].

[1] V. Palchykov, C. von Ferber, R. Folk, and Yu. Holovatch, *A coupled order parameter system on a scale-free network*, preprint arXiv:0903.4759.
[2] V. Palchykov, C. von Ferber, R. Folk, Yu. Holovatch, and R. Kenna, *Critical phenomena on scale-free networks: logarithmic corrections and scaling functions*, preprint arXiv:1004.0097.

A new method of solving inverse problems (P)

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The main idea of the paper 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. The creation

of these populations is governed by dependent genetic processes with low complexity. We present hp-HGS genetic strategy (hp-adaptive Finite Element Method (FEM) combined with HGS) for solving parametric inverse problems. These problems are formulated as the global optimization ones, where the objective is to express the discrepancy between the computed and measured energy or displacement. The efficiency of the proposed strategy results from coupling an adaptive accuracy of solving optimization problems with the accuracy of hp-FEM problem. We apply the method to Step-and-Flash Imprint Lithography, a modern patterning process utilizing photopolymerization to replicate the topography of a template onto a substrate.

Monte Carlo study of the droplet-strip transition in the two-dimensional Ising model (P)

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The 2D Ising model is studied with the constraint of fixed magnetization under half-free/half-periodic boundary conditions below the critical temperature. Depending on the system magnetization, overturned spins prefer to form clusters of approximately semi-circular shape or percolating strips. The transition between these configurations requires the surmounting of a free-energy barrier, which is estimated by histogram analysis and geometric measurement of the saddle-point shape interface length.

Stability and timing in Boolean dynamics

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Regulatory dynamics has mathematical descriptions in terms of rate equations for continuous variables and, after discretization of the state space, as Boolean maps. Here we study this discretization in detail. In particular, we define the stability of a Boolean state sequence in consistency with the stability of the original continuous trajectory that has been discretized. In essence, the stability criterion translates infinitesimal perturbations in the state space of the continuous system into infinitesimal time lags in the Boolean counterpart. For a class of randomly connected systems with randomly drawn Boolean functions, so-called Kauffman networks, we find that the dynamics is stable for almost all choices of parameter values. The so-called "chaotic" regime in Kauffman networks appears only as a damage spreading effect after flip perturbations. We conclude that regulatory systems amenable to state discretization do not exhibit chaotic behaviour.

IBERCIVIS: A BOINC-based platform for scientific computing

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We present a BOINC-based computing infrastructure called IBERCIVIS. It was launched two years ago, being its computing power supplied by volunteers and institutions all around the world. Nowadays more than 2×10^4 volunteers provide about 8×10^3 cores every day. Around ten scientific projects spanning from Medicine to Condensed Matter Physics are using the computer. Apart from the large CPU power, it also represents an opportunity to involve Society in basic scientific research. By using web pages and blogs, every scientific project can present their results in an informal and motivating way. We explain the road map an application must follow to run in IBERCIVIS and, to concrete, we describe the adaptation of a typical spin model code. Finally we give some preliminary numerical results on the diluted Potts model in three dimensions, obtained using the platform.

[1] A. Gordillo-Guerrero, *Phase transitions in disordered systems*, preprint arXiv:1004.1579.

Massively parallelized replica-exchange simulations of polymers on GPUs

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We discuss the advantages of parallelization by multithreading on graphics processing units (GPUs) for parallel tempering Monte Carlo computer simulations of an exemplified bead-spring model for homopolymers. Since the sampling of a large ensemble of conformations is a prerequisite for the precise estimation of statistical quantities such as typical indicators for conformational transitions like the peak structure of the specific heat, the advantage of a strong increase in performance in Monte Carlo simulations cannot be overestimated. Employing multithreading and utilizing the massive power of the large number of cores on GPUs, being available in modern but standard graphics cards, we find a rapid increase of speed-up when porting parts of the code from the central processing unit (CPU) to the GPU.

Large-deviation properties of largest component for random graphs

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Distributions of the size of the largest components are studied numerically for Erdös-Renyi random graphs and two-dimensional percolation, in particular in the large-deviation tail. We access probabilities as small as 10^{-180} by using an artificial finite-temperature (Boltzmann) ensemble. The distributions for the Erdös-Renyi ensemble agree well with previously obtained analytical results. Furthermore, a first-order phase transition at low temperatures T within the artificial ensemble is found.

The thermodynamic Casimir effect in the neighbourhood of the λ-transition: A Monte Carlo study of an improved three-dimensional lattice model

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We discuss the thermodynamic Casimir effect in thin films in the three-dimensional XY universality class. Based on the results of Monte Carlo simulations of an improved lattice model we compute the universal finite-size scaling function θ that characterizes the behaviour of the thermodynamic Casimir force in the neighbourhood of the critical point. Leading corrections to the universal finite-size scaling behaviour due to free boundary conditions can be expressed by an effective thickness $L_{0,\mathrm{eff}} = L_0 + L_s$, with $L_s = 1.02(7)$. We compare with experiments on films of ^{4}He near the λ-transition, previous Monte Carlo simulations of the XY model on the simple cubic lattice and field-theoretic results. Our result for the finite-size scaling function θ is essentially consistent with experiments on films of ^{4}He and previous Monte Carlo simulations.

The thermal Casimir effect in films: Monte Carlo simulations of improved models (P)

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We study the thermodynamic Casimir force for films in the three-dimensional Ising universality class with symmetry breaking boundary conditions. To this end we simulate the improved Blume-Capel model on the simple cubic lattice. We study the two cases $++$, where all spins at the boundary are fixed to $+1$ and $+-$, where the spins at one boundary are fixed to $+1$ while those at the other boundary are fixed to -1. An important issue in analyzing Monte Carlo and experimental data are corrections to scaling. Since we simulate an improved model, leading corrections to scaling, which are proportional to $L_0^{-\omega}$, where L_0 is the thickness of the film and $\omega \approx 0.8$, can be ignored. This allows us to focus on corrections to scaling that are caused by the boundary conditions. We confirm the theoretical expectation that these corrections can be accounted for by an effective thickness $L_{0,\text{eff}} = L_0 + L_s$. Studying the correlation length of the films, the energy per area and the thermodynamic Casimir force at the bulk critical point we find $L_s = 1.9(1)$ for our model and the boundary conditions discussed here. Using this result for L_s we find a nice collapse of the finite-size scaling curves obtained for the thicknesses $L_0 = 8.5$, 16.5 and 32.5 for the full range of temperatures that we consider. We compare our results for the finite-size scaling functions θ_{++} and θ_{+-} of the thermodynamic Casimir force with those obtained in a previous Monte Carlo study, by the de Gennes-Fisher local-functional method, field theoretic methods and an experiment with a binary mixture.

[1] M. Hasenbusch, *Thermodynamic Casimir effect for films in the three-dimensional Ising universality class: Symmetry-breaking boundary conditions*, Phys. Rev. B **82** (2010) 104425-1–15.

Polymer chain stiffness versus excluded volume: A Monte Carlo study of the crossover towards the wormlike chain model

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When the local intrinsic stiffness of a polymer chain varies over a wide range, one can observe both a crossover from rigid-rod-like behavior to (almost) Gaussian random coils and a further crossover towards self-avoiding walks in good solvents. Using the pruned-enriched Rosenbluth method (PERM) to study self-avoiding walks of up to $N_b = 50000$ steps and variable flexibility, the applicability of the Kratky-Porod model is tested. Evidence for non-exponential decay of the bond-orientational correlations $\langle \cos\theta(s) \rangle$ for large distances s along the chain contour is presented, irrespective of chain stiffness. For bottle-brush polymers on the other hand, where experimentally stiffness is varied via the length of side-chains, it is shown that these cylindrical brushes (with flexible backbones) are not described by the Kratky-Porod wormlike chain model, since their persistence length is (roughly) proportional to their cross-sectional radius, for all conditions of practical interest.

[1] H.-P. Hsu, W. Paul, and K. Binder, *Polymer chain stiffness versus excluded volume: A Monte Carlo study of the crossover towards the wormlike chain model*, preprint arXiv:1010.0639, to appear in Europhys. Lett. (in print).

Infinite disorder scaling of random quantum magnets in three and higher dimensions

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Using a very efficient numerical algorithm of the strong disorder renormalization group method we have extended the investigations about the critical behavior of the random transverse-field Ising model in three and in higher dimensions. In all studied cases an infinite disorder quantum critical point is identified, which ensures that the applied method is asymptotically correct and the calculated critical exponents tend to the exact values

for large scales. We have shown that the critical exponents are independent of the form of the disorder and they are smooth functions of the dimensionality.

[1] I. A. Kovacs and F. Iglói, *Infinite disorder scaling of random quantum magnets in three and higher dimensions*, preprint arXiv:1010.2344.

Size matters, except perhaps for pure mathematicians

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We consider groups of interacting nodes engaged in a common activity as many-body, complex physical systems and analyse their cooperative behaviour from a mean-field point of view. We show that inter-nodal interactions rather than accumulated individual node strengths dominate the quality of group activity, and give rise to phenomena akin to phase transitions, where the extensive relationship between group quality and quantity reduces. The theory is applied and tested using empirical data on quantity and quality of academic research groups coming from British and French research evaluation exercises. Contrary to naive expectations that the quality of a research group is simply given by the mean calibre of its individual academics, the analysis indicates that intra-group interactions indeed play a dominant role: the theory is supported. The notion of "critical mass" in research has existed for a long time without precise definition. Our analysis facilitates a definition and we show there are in fact two critical masses in research: a lower one, below which teams are vulnerable and an upper one, above which average dependency of research quality on group size reduces. We determine these critical masses for research groups for various disciplines and indicate how support should be targeted to optimise the national strength of a given discipline.

[1] R. Kenna and B. Berche, *The extensive nature of group quality*, Europhys. Lett. **90** (2010) 58002-1–6 [arXiv:1004.3155].

Statistics beyond physics – misused in public?

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Data collections and statistical investigation require a careful consideration of factual, local and temporal criteria of identification as well as an estimation for the scattering region of single data. When statistics are related to a geographic region, every single event is "proportionally" assigned to the whole region. Only if sufficiently many events exist, which are evenly distributed, the local criterion is fulfilled. Extreme events with temporal and local singularities violate the principle of "self-averaging" of statistics. Hence their evaluation depends on the choice of an arbitrary reference parameter. Results are discussed using the example of murderers and victims of amok in the German police crime statistics.

Spherical polymer brushes under good solvent conditions: Molecular dynamics results compared to density functional theory

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One of the challenging problems in soft matter physics is to characterize from the primary constituents the process of design of polymeric molecules for specific targets. For instance, a thorough understanding of biological materials, such as proteins and drug delivery vehicles, has to take into account the creation of specific macromolecular conformations and structures and the possibility of self-assembly in several processes. A coarse grained model for flexible polymers end-grafted to repulsive spherical nanoparticles is studied for various chain lengths

and grafting densities under good solvent conditions, by Molecular Dynamics methods and density functional theory. With increasing chain length the monomer density profile exhibits a crossover to the star polymer limit. The distribution of polymer ends and the linear dimensions of individual polymer chains are obtained, while the inhomogeneous stretching of the chains is characterized by the local persistence lengths. The results on the structure factor of both single chain and full spherical brush as well as the range of applicability of the different theoretical tools are presented. Finally the polymer dynamics is briefly discussed.

[1] F. Lo Verso, S. A. Egorov, A. Milchev, and K. Binder, *Spherical polymer brushes under good solvent conditions: Molecular dynamics results compared to density functional theory*, preprint `arXiv:1005.0235`.

Worm algorithm in ordered and disordered media (P)

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The Worm algorithm is a Monte Carlo method that uses the high-temperature expansion for simulating spin systems. It was introduced by Prokof'ev and Svistinov in 2001 [1]. This work and a few other papers suggest that it does not suffer from critical slowing down. We investigated the critical behavior of the algorithm, which means we have calculated the dynamic critical exponents. This procedure has also been done for bond-disordered and site-diluted systems, therefore we expanded the algorithm to such systems and introduced several estimators for common observables. We could affirm that the critical slowing down has no practical influence for the Worm algorithm, this also holds for disordered and diluted systems. Furthermore, we have introduced a reweighting method and discussed an estimator which characterizes the spatial correlations of the system.

[1] N. Prokof'ev and B. Svistunov, *Worm algorithm for classical statistical models*, Phys. Rev. Lett. **16** (2001) 160601-1–4.

Formulation of time from Aristotle to Monte Carlo simulations and to noncommutative geometry

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Aristotle defines time as a quantity which can only be derived from motion. In Classical Mechanics time enters as a parameter into the Newtonian equations of motion. In Quantum Mechanics and in Quantum Field Theory time also is a parameter in the Schrödinger or Dirac equation. In Special Theory of Relativity a time dilatation appears, but time stays as a (relative) parameter. The same is the case in General Theory of Relativity, where for some metrics one finds trajectories into the past. The fundamental equations of Physics are invariant with respect to inversion of time. The Second Law of Thermodynamics violates this symmetry and leads to an arrow of time. In Noncommutative Geometry time becomes an operator. In Monte Carlo simulations, the relation between computer time and real time is an interesting question. Using atomic clocks, time and frequency are the most precisely measurable observables. An overview of time in different fields of physics is given.

Critical behavior of three-dimensional disordered Potts models with many states

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We study the 3D disordered Potts model with $p = 4$, 5 and 6 (being p the number of states). We have used the special purpose supercomputer JANUS, so we managed to simulate sizes up to $L = 12$ and 16 with lengths up

to 10^{11} MCS. Our numerical simulations (that severely slow down for increasing p) detect a very clear spin-glass phase transition. We evaluate the critical exponents and the critical value of the temperature, and we use known results at lower p values to discuss how they evolve for increasing p. We discuss the possible scenarios for large p values, considering a (disordered) first-order phase transition, in particular for $p = 10$ which is relevant for the glass transition. Finally, we do not find any sign of the presence of a transition to a ferromagnetic regime in the spin-glass critical region.

[1] R. Alvarez Banos *et al.*, *Critical behavior of three-dimensional disordered Potts models with many states*, JSTAT (2010) P05002-1–16.
[2] A. Cruz *et al.*, *The spin-glass phase in the four-state, three-dimensional Potts model*, Phys. Rev. B **79** (2009) 184408-1–6 [arXiv:0812.1287].

A new ansatz for thermodynamics of confined systems

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Over the last few years, we have worked out a new theory for "Thermodynamics of Confined Systems". A first application of this theory has been shown to explain some key experiments in the field of fluids in mesopores [1]. A short outline of the developed new theory and the motivation for its development will be presented at the workshop. Even though several aspects of the theory are still in the make it appears justified to expect that standard thermodynamics can be understood as a limiting case of confined thermodynamics. Further, it appears that nucleation in macroscopic systems can be treated in within the concepts of the new theory: as nucleation occurs in a small volume of a macroscopic system, the separation into a small subsystem and a large environment with constant properties is conceptually possible. The problem of how to select the volume of the subsystem will be discussed. It turns out that the appropriate size can be read off the calculations and, thus, is not arbitrary. A part of the talk is devoted to the potential for practical use. It turns out that the new theory does not only remove conceptual problems, but at the same time opens the route to a number of new states found in confined (porous) systems which may lead to improved applications. In particular we will focus on the possibility to drive a fluid in a pore into exotic states under static and under dynamic conditions. E.g., it turns out that states with negative pressure can be reproducibly controlled. Negative pressure states are in principal known since the time of Torricelli and they have been discussed in the literature [2, 3] as experimentally accessible situations. Still, they have not been turned into practical usefulness which is likely to be caused by the notion of their metastability in macroscopic systems.

[1] H. Morgner, *Computer simulation on static and dynamic properties during transient sorption of fluids in mesoporous materials*, J. Phys. Chem. C **114** (2010) 8877–8883.
[2] A. R. Imre, *On the existence of negative pressure states*, Phys. Stat. Sol. (b) **244** (2007) 893–899.
[3] A. R. Imre *et al.*, *Indirect methods to study liquid-liquid miscibility in binary liquids under negative pressure*, NATO Science Series II, Mathematics, Physics and Chemistry (2007) **242**: *Soft Matter under Exogenic Impacts*, pp. 389–398.

Towards optimized parallel tempering (P)

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Parallel tempering Monte Carlo methods are an important tool for numerical studies of models with large complexity, since interesting questions, like the origin of phase transitions and structure formation, can only be tackled by means of statistical analysis. For the efficient implementation when using many-core architectures, different optimizations on the distribution of the inverse temperatures are studied. A method of replicated temperature partitions is proposed and tested using the well-known Ising model.

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Condensation time scale of a stochastic transport process with pair factorized steady states (P)

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Stochastic transport processes (such as [1]) can be tuned by their generating weight functions to exhibit a steady state with a condensate of particles that is separate from a fluid background phase. We study the dynamics of the relaxation into the steady state of such driven transport systems using numerical simulations to determine the condensation time scale and discuss the corresponding phenomenologic mechanisms. Despite the existence of short-range interactions in the studied system, the condensation behavior is found to be quite similar to that of the zero-range process on one- and two-dimensional lattices.

[1] M. R. Evans, T. Hanney, and S. N. Majumdar, *Interaction driven real-space condensation*, Phys. Rev. Lett. **97** (2006) 010602-1–4
[2] H. Nagel, *Mass Condensation in Stochastic Transport Processes and Complex Networks*, Diploma thesis, Leipzig (2010).

More on quantum adiabatic computations

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We determine the classical and quantum complexities of a specific ensemble of three-satisfiability problems with a unique satisfying assignment for up to $N = 100$ and $N = 80$ variables, respectively. In the classical case we employ generalized ensemble techniques and measure the time that a Markovian Monte Carlo process spends in searching classical ground states. In the quantum case we determine the maximum finite correlation length along a quantum adiabatic trajectory that uses constant transverse field. In the median of our ensemble both complexities diverge exponentially with the number of variables. Hence, adiabatic quantum computation fails to reduce intractable classical complexity to a polynomial one. Moreover, the growth-rate constant of the quantum case is 3.8 times as large as the one of the classical case, making classical fluctuations more beneficial than quantum fluctuations in ground-state searches.

Gibbs-Thomson effect in the Ising model (P)

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We investigated for the Ising model the influence of a curved surface on the ambient pressure which is known as the Gibbs-Thomson effect. To this end, we performed extensive numerical studies in two and three dimensions at different temperatures of the next-neighbor lattice, which nicely agree with theoretical predictions from Biskup *et al.* [1].

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Anisotropic Heisenberg antiferromagnets

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We study classical and quantum Heisenberg antiferromagnets with exchange anisotropy of XXZ-type and crystal field single-ion terms of quadratic and cubic form in a field. The magnets display a variety of phases, including the spin-flop (or, in the quantum case, spin-liquid) and biconical (corresponding, in the quantum lattice gas description, to supersolid) phases. Applying ground-state considerations, Monte Carlo and density matrix renormalization group methods, the impact of quantum effects and lattice dimension is analysed. Interesting critical and multicritical behaviour may occur at quantum and thermal phase transitions.

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Ising spin-glass transition in magnetic field out of mean-field: Numerical simulations and experiments

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The existence of a spin-glass transition in presence of a magnetic field is one of the most challenging problems, both in theory as in experiments, in the field of disordered systems. We have addressed this problem by simulating the one-dimensional Ising spin glass with power-law decay in the couplings. There exists a matching between this model and finite-dimensional Ising spin glasses with short-range couplings. By simulating different values of the power-law decay exponent, we can change the dimensionality of the (equivalent) finite-dimensional (short ranged) spin glass. Using a new finite-size scaling method, we have numerically obtained clear signatures of a paramagnetic–spin-glass phase transition in presence of an external magnetic field for values of the power-law decay exponent which correspond with dimensions well below the upper critical dimension of the Ising spin glass. In addition we have conjectured that the phase transition could be observed in experiments in the regime of low magnetic fields (below 1000 Oe). Finally, we will discuss our findings in the light of old and new experiments.

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On the low-temperature behavior of a geometrically frustrated Heisenberg antiferromagnet*

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The Heisenberg antiferromagnet on the (two-dimensional) kagome lattice has been subject of numerous studies in the past two decades, and today its thermodynamic behavior is widely understood. In the kagome geometry each spin belongs to two spin triangles, hence the system is highly frustrated. At low temperatures one observes ordering by disorder [1], i.e. planar spin configurations due to multiple zero-modes, the so-called Weathervane loops, are favored entropically. These modes occur when spin clusters are bounded by spins pointing in a similar direction, thus allowing the cluster spins to revolve freely around this direction. However, it remains unclear if with decreasing temperature the number of these modes continues to increase and if this eventually leads to the highly ordered $\sqrt{3}\times\sqrt{3}$ state. To answer this question we have performed extensive Monte Carlo simulations of the Heisenberg kagome antiferromagnet. We applied the simulated tempering method [2], with the dynamics for the canonical subensembles provided by the Heatbath algorithm [3] for single spins and a Metropolis loop-flip Monte Carlo move. We were able to examine the thermodynamic properties for temperatures $10^{-6} \leq k_{\mathrm{B}}T/J \leq 10^{3}$

with J being the nearest-neighbor interaction constant; and we find that once the planar state is attained at $k_{\rm B}T/J \approx 10^{-2.6}$, the out-of-plane excitations are reduced with decreasing temperature but no further order is established. This indicates that the prevailing spin structure represents a temperature independent entropy maximum where any entropy gain produced by additional zero modes is neutralized by an entropy loss in the Weathervane loop structure.

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Domain walls and Schramm-Loewner evolution in the random-field Ising model

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The concept of Schramm-Loewner evolution provides a unified description of domain boundaries of many lattice spin systems in two dimensions, possibly even including systems with quenched disorder. Here, we study domain walls in the random-field Ising model. Although, in two dimensions, this system does not show an ordering transition to a ferromagnetic state, in the presence of a uniform external field spin domains percolate beyond a critical field strength. Using exact ground-state calculations of very large disorder samples, we examine ground-state domain walls near this percolation transition finding strong evidence that they are conformally invariant and satisfy the domain Markov property, implying compatibility with Schramm-Loewner evolution (SLE_κ) with parameter $\kappa = 6$. These results might pave the way for new field-theoretic treatments of systems with quenched disorder.

Optimizing Wilson's momentum shell renormalization group

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Previous attempts to accurately compute critical exponents from Wilson's momentum shell renormalization prescription suffered from the difficulties posed by the presence of an infinite number of irrelevant couplings. Taking the example of the 1d long-ranged Ising model [1], we calculate the momentum shell renormalization flow in the plane spanned by the coupling constants (u_0, r_0) by a simulation method based on our recently developed Fourier Monte Carlo algorithm [2, 3]. Carrying out such simulations for different values of the momentum shell thickness parameter b, we report [4] strong anomalies in the b-dependence of the fixed point couplings and the resulting exponents y_τ and ω in the vicinity of a shell parameter $b^* < 1$ characterizing a thin but finite momentum shell. Evaluation of the exponents for this "optimized" value b^* of b yields a dramatic improvement of their numerical accuracy, indicating a strong damping of the influence of irrelevant couplings.

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Performance potential for simulating spin models on GPU

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Over the last couple of years it has been realized that the vast computational power of graphics processing units (GPUs) could be harvested for purposes other than the video game industry. This power, which at least nominally exceeds that of current CPUs by large factors, results from the relative simplicity of the GPU architectures as compared to CPUs, combined with a large number of parallel processing units on a single chip. To benefit from this setup for general computing purposes, the problems at hand need to be prepared in a way to profit from the inherent parallelism and hierarchical structure of memory accesses. In this contribution I discuss the performance potential for simulating spin models, such as the Ising or Heisenberg models as well as the Edwards-Anderson spin glass, on GPU as compared to conventional simulations on CPU. Different algorithms, including Metropolis [1] and cluster updates [2], as well as computional tricks such as multi-spin coding are taken into account.

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Critical properties of the 120 degree model for orbital ordering

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"Orbital only" spin models are the simplest models to describe the interplay of orbital degrees of freedom in transition metal oxids. These orbital models possess many interesting features not present in ordinary spin models of magnetism and have currently generated a considerable amount of interest in condensed matter physics. One of the paradigm example in these class of models is the so called eg-orbital model (or 120 degree model), for which a long-range ordered phase was only recently established mathematically. We have performed a dedicated Monte Carlo analysis of this finite-temperature phase transition and I will report in this talk on its nature and critical properties.

Monte Carlo test of the classical theory for heterogeneous nucleation

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Nucleation is a ubiquitous process which governs such diverse phenomena as the formation of rain drops or snow flakes in the atmosphere, the crystallization of proteins and even the formation of industrially relevant polymer foams. Even though considerable empirical knowledge has been gathered, e.g., on which materials are suited as seed particles for making clouds rain or as nucleation agents to start precipitation in metallurgy, many questions remain. Nucleation is typically enhanced by the presence of a wall in the system. The free energy of a droplet in contact with a wall is reduced in comparison to the free energy of a droplet in the bulk. The difference between the homogeneous and the heterogeneous case can be described by Turnbull's formula which determines the free energy of a droplet as a function of the contact angle given by Young's equation. In this work, we test this classical formula with Monte Carlo simulations of the 3d Ising model.

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Atomistic molecular dynamics simulations of polybutadiene at graphite: Wall impact on polymer statics and dynamics

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A nanoscopic thin polybutadiene film confined between two graphite surfaces is studied by MD simulations of an atomistic model. Various analysed properties, e.g., profiles of density, gyration radii, bond and molecule orientations as well as corresponding time-correlation functions show an influence of confinement on the polymer property in a wide range of scales.

Model gene regulatory networks under mutation-selection balance

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Gene regulatory networks typically have low in-degrees, whereby any given gene is regulated by few of the genes in the network. They also tend to have broad distributions for the out-degree. What mechanisms might be responsible for these degree distributions? Starting with an accepted framework of the binding of transcription factors to DNA, we consider a simple model of gene regulatory dynamics. There, we show that selection for a target expression pattern leads to the emergence of minimum connectivities compatible with the selective constraint. As a consequence, these gene networks have low in-degree, and *functionality* is parsimonious, i.e., is concentrated on a sparse number of interactions as measured for instance by their essentiality. Furthermore, we find that mutations of the transcription factors drive the networks to have broad out-degrees. Finally, these classes of models are evolvable, i.e., significantly different genotypes can emerge gradually under mutation-selection balance.

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Copulas applied in the inverter case study (P)

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The inverter operational data is analysed with a goal to derive dependencies between occurrence of unwanted peak in frequency domain of motor speed signal and statistical characteristics of the data. In order to infer possible relations we apply copula theory, which is a general way of describing various dependencies between random variables. For initial analysis we apply graphical and numerical rank-based methods. We consider a family of Archimedean copulas with a special focus on the Gumbel-Hougaard and Clayton copulas. The parameter estimation is performed with maximum pseudolikelihood method and estimators based on Kendall's tau. Final results are tested for goodness-of-fit, and it is concluded that Gumbel-Hougaard copula reflects the dependencies in the investigated data sample better than the Clayton copula.

Structure of the Tip4p model in the ice I_h phase (P)

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Potential water models have been widely used throughout the last decades in a variety of computer simulations. Especially in the simulations of processes where water is used as a solvent, the influence of the model is easily underestimated and can provide a large source of error. We investigated the behavior of the Tip4p model with different parametrizations in the hexagonal, ordinary ice phase. To this end random spherical nanosized water clusters were arranged in the experimentally determined tetrahedral structure. These configurations were minimized in energy with a semi-dynamic technique, resulting in local energy minimium configurations of the specific water model. Important to notice is the necessity of the correct consideration of the involved long-range interactions, especially the electrostatic one which cannot be handled trivially by a cutoff. This process revealed insight into the properties of the model near and in the ice phase, confirming the stability of the hexagonal structure with multiple local minima, with almost identical energies. That way the principle structure of the unit cell was obtained and compared for the different parameterizations. The influence on Monte Carlo simulations is currently investigated.