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ABSTRACTS

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Abstracts

Exact ground states in $6d$ random-field Ising magnets

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We calculate exact ground states of random-field Ising magnets (RFIM) in 6 dimensions up to lattice sizes of $L = 10$. We calculate some critical exponents and compare them with previously obtained mean-field exponents.
The RFIM is a disordered system. It consists of ferromagnetically coupled Ising spins with an additional quenched local magnetic field. Here the field is Gaussian distributed with a fixed mean = 0 and a tunable standard deviation.
To obtain a ground state of a realisation of the disorder we map the random field to a graph with suitible chosen edge capacities [Picard and Ratliff, 1975]. For these graphs we calculate the maximum flow using a fast max-flow/min-cut algorithm, recently developed in algorithmic graph theory. The minimum cut corresponds to a ground state configuration of the system. We can measure the bond energy, the magnetisation and the susceptibility by applying a small external field. Using finite-size scaling we can calculate the specific heat exponent α, the order parameter exponent β, the susceptibility exponent γ and the correlation length exponent ν. They are compared with the mean-field exponents of the RFIM, because $d_u \leq 6$ is the upper critical dimension [Tasaki, 1989] from which on the mean-field exponents should hold.

Balance during Wang-Landau recursion simulations

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Wang-Landau method is generally considered to be an efficient Monte Carlo algorithm. It certainly is an easily implemented method to determine the density of states which is required for simulations on generalized ensembles such as multicanonical simulations. But since the Wang-Landau method uses strongly fluctuating, time-dependent weights instead of a fixed ensemble, there is no mathematical proof that the method yields reliable results. This work provides a scheme to evaluate statistical data from time series lacking a fixed ensemble. The scheme is applied to Wang-Landau simulations of the two-dimensional Ising model measuring the energy and magnetization. The results are compared with data from exact enumerations on small lattices as well as with the exact Beale solution and magnetization data from multicanonical simulations for lattice sizes up to 64×64 to check for systematic errors of the algorithm. Additionally, the Wang-Landau method is combined with the Transition Matrix evaluation scheme by Wang and Swendsen to find a good working estimate of the density of states even faster.

Formation of a plateau in the twist order parameter of the bond alternating antiferromagnetic $S = 1/2$ Heisenberg spin chain

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The twist order parameter was introduced in [1] to signal a quantum phase transition between different valence bond configurations in various 1D quantum spin systems. We present quantum Monte Carlo simulations combined with quantum reweighting methods. At non-zero temperature we find the formation of a plateau in the twist order parameter around the (zero temperature) quantum critical point. We investigate the possibility that this plateau is related to the quantum critical region that fans out from the quantum critical point.

[1] M. Nakamura and S. Todo, Phys. Rev. Lett. **89**, 077 204 (2002).

Replica-exchange cluster algorithm

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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.

Random walks on percolation clusters: multifractal effects

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We consider self-avoiding walks (SAWs) on the backbone of percolation clusters, having a fractal structure, in space dimensions $d = 2$, 3, and 4. Applying numerical simulations, we show that the conventional scaling can not completely describe the system, and the whole multifractal spectrum of singularities emerges in exploring these peculiarities. We obtain estimates for the set of critical exponents, that govern scaling laws of higher moments of the distribution of percolation cluster sites visited by SAWs, in a good correspondence with recent field-theoretical $\varepsilon = 6 - d$-expansion.

Ageing in bosonic contact and pair-contact processes with Lévy flights: exact results

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Ageing in systems without detailed balance is studied in bosonic contact and pair-contact process with Lévy diffusion. In the ageing regime, the dynamical scaling of the two-time correlation function and two-time response function is found and analyzed. Exacts results for exponents and scaling functions are derived. The behaviour of the fluctuation-dissipation ratio is analyzed and compared to spherical model one and a crossing time from relaxation regime to ageing regime is defined.

On computing the partition function for the Potts model with many states

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The partition function of the q-state Potts model with random ferromagnetic couplings and large q amounts to minimizing a particular submodular function. Combinatorial optimization algorithms with polynomial running time exist for minimizing a general submodular function. However, in practice the running time of these algorithms grows strongly with the system size. Thus only relatively small instances can be computed. In our case, faster specialized algorithms can be used. We investigate several approaches to further improve these algorithms in order to reach better average running times.

Strong coupling QCD as a dimer model

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The dimer formulation of QCD at strong coupling is reviewed and recent results of the phase diagram are presented.

Ultrametricity and clustering of states in spin glasses: a one-dimensional view

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We present results from Monte Carlo simulations to test for ultrametricity and clustering properties in spin-glass models. By using a one-dimensional Ising spin glass with random power-law interactions where the universality class of the model can be tuned by changing the power-law exponent, we find signatures of ultrametric behavior both in the mean-field and non-mean-field universality classes for large linear system sizes. Furthermore, we confirm the existence of nontrivial connected components in phase space via a clustering analysis of configurations.

Kosterlitz-Thouless transition of thin films in the 3D XY universality class

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We study thin films in the XY universality class. To this end, we perform a Monte Carlo study of the improved ϕ^4-model on the simple cubic lattice. We study films of a thickness up to $L_0 = 32$ lattice spacings. In the short direction of the lattice free boundary conditions are employed. Using a particular finite size scaling (FSS) method, proposed recently, we determine the temperature of the Kosterlitz-Thouless transition with high accuracy. The finite size scaling behaviour of the Binder cumulant U_4, the second moment correlation length over the lattice size ξ_{2nd}/L, the ratio of the partition functions with periodic and anti-periodic boundary conditions Z_a/Z_p and the helicity modulus Υ clearly confirm the KT-nature of the transition. Next we analyse the scaling of the KT-transition temperature with the thickness of the film. The predictions of the renormalization group (RG) theory are confirmed. We compute universal ratios of the thickness of the film L_0 with the correlation length in the infinite volume at KT-transition temperature. These results can be compared with experimental results on thin films of ^{4}He near the λ-transition.

Kinetics of a non-glauberian Ising model: exact results

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The spin-flip dynamics in kinetic Ising chains with Kimball-Deker-Haake (KDH) transition rates is analysed. Exact closed equations of motion for global quantities such as the magnetization and its fluctuations, and the two-time susceptibilities of total spin and three-spin are derived and solved. Non-equilibrium exponents relevant for ageing behaviour are extracted.

Structure of bottle-brush polymers in solutions: a Monte Carlo study

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Bottle-brush polymers with a rigid backbone and flexible side chains are studied in a good solvent and a theta solvent. They are simulated by using a coarse-grained model on a simple cubic lattice with Monte Carlo simulations. Varying the side chain length, backbone length, and the grafting density, the scaling behavior of the radius of gyration, end-to-end distance, radial density profiles of monomers and side chain ends are estimated and checked with the previous theoretical predictions [1]. In order to compare our results with experimental scattering data, the structure factors describing the scattering from a single side chain and from the total bottle-brush polymer are also estimated. Our simulations include two sets of data: (1) To describe the structure of a very long bottle-brush polymer, a periodic boundary condition along the backbone is used. (2) To describe effects due to the finiteness of the backbone, free ends of the backbone are considered in our simulations. In the latter case, the inhomogeneity of the structure in the direction along the backbone is carefully investigated. With our simulation results we test various phenomenological models that have been proposed to interpret experimental scattering data for bottle-brush polymers. A detailed analysis of radial density profile and the total scattering of a bottle-brush are given.

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[2] H.-P. Hsu, W. Paul, and K. Binder, arXiv:0808.1485; to appear in J. Chem. Phys. (2008, in press).

Nonequilibrium critical dynamics of the two-dimensional Ising model quenched from a correlated initial state

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The universality class, even the order of the transition, of the two-dimensional Ising model depends on the range and the symmetry of the interactions (Onsager model, Baxter-Wu model, Turban model, etc.), but the critical temperature is generally the same due to self-duality. Here we consider a sudden change in the form of the interaction and study the nonequilibrium critical dynamical properties of the nearest-neighbor model. The relaxation of the magnetization and the decay of the autocorrelation function are found to display a power law behavior with characteristic exponents that depend on the universality class of the initial state.

Information geometry and phase transitions

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The idea of using differential geometry in thermodynamics has been pursued by, notably, Weinhold and Ruppeiner who introduced metric structures in the space of equilibrium states. Phase transitions are discernible as curvature singularities. There has been a burst of recent activity, with conflicting results, on applying the ideas to black hole phase transitions. We discuss the background to the theory and some of the unresolved puzzles.

Comparative atomistic and coarse-grained study of water: simulation details vs. simulation feasibility

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We employ the inverse Boltzmann method to coarse-grain three commonly used three-site water models (TIP3P, SPC and SPC/E) where one molecule is replaced by one coarse-grained particle with two-body interactions only. The shape of the coarse-grained potentials is dominated by the ratio of two lengths, which can be rationalized by the geometric constraints of the water clusters. It is shown that for simple two body potentials either the radial distribution function or the geometrical packing can be optimized. In a similar way, as needed for multiscale methods, either the pressure or the compressibility can be fitted to the all atom liquid. In total, a speedup of a factor of about 50 in computation time can be reached by this "coarse-gaining" procedure.

Out-of-equilibrium bosons on a one-dimensional optical random lattice

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We study the transport properties of a one-dimensional hard-core boson lattice gas coupled to two particle reservoirs at different chemical potentials generating a current flow through the system. In particular, the influence of random fluctuations of the underlying lattice on the stationary state properties are investigated. We show analytically that the steady-state density presents a linear profile. The local steady-state current obeys the Fourier law $j = -\kappa(\tau)\nabla\rho$ where here τ is a typical time-scale of the lattice fluctuations and $\nabla\rho$ the density gradient imposed on the system by the reservoirs.

Scaling analysis of the site-diluted Ising model in two dimensions

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A combination of numerical and analytical advances are applied to analyze the scaling behaviour of the site-diluted Ising model in two dimensions, paying particular attention to the multiplicative logarithmic corrections in that model. The analysis focuses primarily on the odd sector, and in particular on Lee-Yang zeros, which are determined to high accuracy. Scaling relations for logarithmic corrections are used to connect to the even sector, and a first analysis of the density of zeros yields information on the specific-heat. The analysis is supportive of the strong scaling hypothesis and scaling relations for logarithmic corrections are verified.

Tethered Monte Carlo: computing the effective potential without critical slowing down

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We present Tethered Monte Carlo, a simple, general purpose method of computing the effective potential of the order parameter (Helmholtz free energy). This formalism is based on a new statistical ensemble, closely related to the micromagnetic one, but with an extended configuration space (through Creutz-like demons). Canonical averages for arbitrary values of the external magnetic field are computed without additional simulations. The method is put to work in the two-dimensional Ising model, where the existence of exact results enables us to perform high precision checks. A rather peculiar feature of our implementation, which employs a local Metropolis algorithm, is the total absence, within errors, of critical slowing down for magnetic observables. Indeed, high accuracy results are presented for lattices as large as $L = 1024$.

Scaling behavior of domain walls at the $T = 0$ ferromagnet to spin-glass transition

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Using mappings to combinatorial optimization problems, one can often study physical systems better by means of sophisticated algorithms from computer science. Here, we study the geometric properties of domain-wall excitations in a two-dimensional random-bond Ising spin system, where each realization of the disorder consists of a random fraction ρ of ferromagnetic bonds and a fraction $(1-\rho)$ of bonds drawn from a Gaussian distribution with zero mean and unit width. We formulate an auxiliary graph theoretical problem in which domain walls are given by undirected shortest paths with possibly negative distances [1]. Due to the details of the mapping, standard shortest path algorithms (e.g. the Dijkstra algorithm) cannot be applied. To solve such shortest path problems it requires minimum weight perfect matching algorithms. We first locate the critical point ρ_c, where the ferromagnet (large ρ) to spin-glass transition occurs. For certain values of ρ close to the critical point we investigate the stiffness exponent θ and the fractal dimension d_f that describe the scaling of the average domain-wall energy and length, respectively. Performing a finite-size scaling analysis we find that both exponents remain constant in the spin-glass phase, i.e. $\theta \approx -0.28$ and $d_f \approx 1.275$. This is consistent with conformal field theory, where it seems to be possible [2] to relate the exponents via $d_f - 1 = 3/[4(3+\theta)]$.

[1] O. Melchert and A.K. Hartmann, Phys. Rev. B **76**, 174411 (2007).
[2] C. Amoruso, A.K. Hartmann, M.B. Hastings, and M.A. Moore, Phys. Rev. Lett. **97**, 267202 (2006).

Quantitative prediction of the phase diagram of alkanes in polar solvents

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The prediction of the equation of state and phase behavior of simple polar fluids and their mixtures with short alkanes is discussed by Monte Carlo computer simulation and an analytical equation of state. Alkanes are modelled using established techniques in which every three carbon units are mapped in a single bead interacting with Lennard-Jones potentials with other beads plus a confining FENE potential between neighbor beads along the chains. Solvent molecules are mapped in single beads neglecting all the atomistic detail. In a previous attempt simple LJ potentials were used to fit the solvent potentials. However the model was not able to reproduce properly mixture phase diagrams without strong modifications of the simple Lorentz-Berthelot (LB) combining rules. We introduce a very efficient coarse grained model for simple quadrupolar molecules which is able to reproduce the phase diagram of the single component in excellent agreement with experimental results, also if compared to more realistic atomistic models. In the present investigation we discuss the improvement in the description of the phase diagram of mixture using the new model for the polar solvents. In particular we clarify that the big violations of the LB combining rule used previously are not necessary if the new model for quadrupolar solvents is used. In order to understand (small) residual discrepancies of the actual modeling with experimental results we study also mixture of alkanes in apolar solvents. Following a similar approach, some mixture with dipolar solvents have also been investigated.

Some properties of polymers with tube constraint

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We present findings on the properties of low temperature ground states and thermodynamic properties of polymers with explicit thickness. As a function of the tubes thickness we observe secondary structures like helices, turns, ringlike conformations and rods. We also present first preliminary results on the abundance of knots in thick polymers with secondary structure formation.

Free-energy barriers of spin glass

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In this talk I will present some details how we investigated the Sherrington-Kirkpatrick (SK) mean field model and the Edwards-Anderson (EA) nearest-neighbor spin-glass model by means of Monte Carlo simulations, employing a combination of the multioverlap algorithm with the parallel tempering method. Results of our investigation of the finite-size scaling behaviour of the free-energy barriers which are visible in the probability density of the Parisi overlap parameter are given. Assuming that the mean barrier height diverges with N, the number of spins, as N^{α}, I show, that our data for the SK model is in good agreement with the theoretical value $\alpha = 1/3$. This is then compared to the scaling behaviour to the data from the EA model.

Kagome lattice structures with charge degrees of freedom

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While the magnetic properties of geometrically frustrated lattices have for some time received wide interest, the charge degrees of freedom of such systems have not been as yet so thoroughly studied. For a model of spinless fermions on a 2D checkerboard lattice, it has been shown that fractional charge excitations occur at certain filling factors [1]. Further work has shown that these fractional charges are linearly confined [2]. However, the nature of the confinement on kagome lattices at certain fillings is not yet so well understood. We address this problem through the use of the exact diagonalization method and the numerical calculation of the spectral functions for a model of spinless fermions at 1/3 filling on finite kagome lattices. We present our findings in relation to a quantum dimer model on the hexagonal lattice [3]. We discuss the implications of our calculations with respect to the nature of the dynamics of the fractional charge excitations. We mention briefly related work which seeks to compare the theoretical model with experimental observations of charged-ordered states in materials with kagome lattice structure [4].

[1] P. Fulde, K. Penc, and N. Shannon, Annalen der Physik (Leipzig) **11**, 892 (2002).
[2] F. Pollmann and P. Fulde, EPL **75**, 133 (2006).
[3] R. Moessner, S.L. Sondhi, and P. Chandra, Phys. Rev. B **64**, 144416 (2001).
[4] T. Osaka *et al.*, Phys. Stat. Sol (b) **241**, 61 (2004).

Crystallization of elastic flexible polymers

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We investigated a flexible off-lattice homopolymer, modeled with FENE (finitely extensible nonlinear elastic) bond potential and intramonomeric Lennard-Jones interaction by means of multicanonical Monte Carlo sampling. Considering liquid- and solid-like conformations at low temperatures and corresponding transitions the system exhibits wide similarities to unbound atomic Lennard-Jones clusters. We developed a new method for geometrical classification of competing states and adapted the simulation technique to investigate solid-solid transitions between them. Finally grand-multicanonical simulations were performed in order to understand the size dependence of the polymer's behavior.

Anisotropic three-dimensional Heisenberg antiferromagnets in a field

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Classical Heisenberg antiferromagnets with uniaxial exchange and a cubic anisotropy term in a field are studied, using mainly Monte Carlo techniques. Especially, we analyze the role of non-collinear structures of biconical type occurring in addition to the well-known antiferromagnetic and spin-flop structures. An outlook to DMRG calculations of related quantum models is given.
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Monte Carlo simulation of fluid phase equilibria in square-well fluids: from bulk to two-dimensional layers

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We study the influence of geometric restrictions on vapour/liquid equilibria and critical data of square-well fluids by canonical Monte Carlo simulations. Starting with the three-dimensional bulk fluid we model the confinement by a series of slit-like pores with decreasing slit widths arriving finally at the planar (two-dimensional) fluid layer. We perform virtual particle insertions to estimate chemical potential versus density isotherms and discuss system size effects on the simulation results. To study the influence of the confinement not only on chemical potentials but also on coexistence properties we estimate vapour/liquid coexistence densities applying an equal-area rule to the subcritical chemical potential isotherms. Critical point data are calculated from the coexistence densities by means of scaling relations. We study the change of the critical temperature and critical density by varying the slit width including the two- and three-dimensional bulk fluids as limiting cases. We find the difference between the bulk and the slit critical temperature to decay exponentially with an exponent reciprocal to a linear function in the slit width. This relation describes accurately both our results [1] and recent findings of critical temperature shift data [2]. No comparable simple relation describing the influence of the confinement on the critical density seems to exist.

[1] H.L. Vörtler, K. Schäfer, and W.R. Smith, J. Phys. Chem. B **112**, 4656 (2008); H.L. Vörtler, Collect. Czech. Chem. Commun. **73**, 518 (2008).
[2] J.K. Singh and S.K. Kwak, J. Chem. Phys. **126**, 024702 (2007).

Localization of maximal entropy random walk

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We define a new class of random walk processes which maximize entropy. This maximal entropy random walk is equivalent to generic random walk if it takes place on a regular lattice, but it is not if the underlying lattice is irregular. In particular, we consider a lattice with weak dilution. We show that the stationary probability of finding a particle performing maximal entropy random walk localizes in the largest nearly spherical region of the lattice which is free of defects. This localization phenomenon, which is purely classical in nature, is explained in terms of the Lifshitz states of a certain random operator.

Extended scaling in high dimensions

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We apply and test the recently proposed "extended scaling" scheme in an analysis of the magnetic susceptibility of Ising systems above the upper critical dimension. The data are obtained by Monte Carlo simulations using both the conventional Wolff cluster algorithm and the Prokof'ev-Svistunov worm algorithm. As already observed for other models, extended scaling is shown to extend the high-temperature critical scaling regime over a range of temperatures much wider than that achieved conventionally. It allows for an accurate determination of leading and sub-leading scaling indices, critical temperatures and amplitudes of the confluent corrections.

Cross-correlations in scaling analyses of phase transitions

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Thermal or finite-size scaling analyses of importance sampling Monte Carlo time series in the vicinity of phase transition points often combine different estimates for the same quantity, such as a critical exponent, with the intent to reduce statistical fluctuations. We point out that the origin of such estimates in the same time series results in often pronounced cross-correlations which are usually ignored even in high-precision studies, generically leading to significant underestimation of statistical fluctuations. We suggest to use a simple extension of the conventional analysis taking correlation effects into account, which leads to improved estimators with often substantially reduced statistical fluctuations at almost no extra cost in terms of computation time.

Dimerized Heisenberg models

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I will talk about quantum phase transitions and critical exponents in a special class of 2D quantum Heisenberg antiferromagnets. In particular, I discuss recent quantum Monte Carlo results on the "staggered" dimerized Heisenberg model. By a detailed comparison to other dimerized models, it is shown, contrary to the current belief, that the critical exponents of the staggered model are most likely not in agreement with the 3D classical Heisenberg universality class. I will also present further thermodynamic studies in the quantum critical region which reinforce these findings.

Monte Carlo simulations of the directional-ordering transition in the classical and quantum compass model in two dimensions

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We report on a comprehensive study of the compass model on the square lattice for classical and quantum spin degrees of freedom using Monte Carlo and Quantum Monte Carlo methods. We employ state-of-the-art implementations using Metropolis, Stochastic Series Expansion and Parallel Tempering techniques to obtain the critical ordering temperatures and critical exponents. In a pre-investigation we reconsider the classical compass model where we study and contrast the finite-size scaling behaviour of ordinary periodic boundary conditions against annealed boundary conditions. We show that periodic boundary conditions suffer from extreme finite-size effects which might be caused by closed loop excitations wrapping around the torus. These excitation also appear to have severe effects on the Binder parameter. On this footing we report on the first systematic Monte Carlo study of the quantum compass model. Our numerical results are at odds with a recent Letter and we trace back the discrepancy to neglecting the finite-size effects on periodic lattices. The data analysis supports a transition in the 2D Ising universality class for both the classical and the quantum model.

Optimized broad-histogram ensembles for the simulation of quantum systems

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The efficiency of statistical sampling in broad-histogram Monte Carlo simulations can be improved by optimizing the simulated extended ensemble for fast equilibration. Here we describe how a recently developed feedback algorithm can be generalized to find optimized sampling distributions for the simulation of quantum systems in the context of the stochastic series expansion (SSE) when defining an extended ensemble in the expansion order. If the chosen update method is efficient, such as non-local updates for systems undergoing a second-order phase transition, the optimized ensemble is characterized by a flat histogram in the expansion order if a variable-length formulation of the SSE is used. Whenever the update method suffers from slowdown, such as at a first-order phase transition, the feedback algorithm shifts weight towards the expansion orders in the transition region, resulting in a non-uniform histogram.

Nonequilibrium spin glass dynamics with Janus

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Janus, the fastest computer ever for simulating discrete spin models in statistical mechanics, entered into full operation March 11, 2008. We simulate the non-equilibrium dynamics of the Ising spin glass. Specifically, we follow the evolution of the Edwards-Anderson model on large lattices for a time that spans eleven orders of magnitude, thus making contact with the experimentally relevant time-scale (i.e. seconds). By studying overlap equivalence and the replicon correlator, we obtain clear evidence for a non-coarsening behavior of the spin-glass in the experimentally relevant times.

Phase transitions in spin glasses

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Whereas there has been a general consensus for some time that Ising spin glasses have a transition at finite temperature in zero field in three dimensions, there has not been general agreement on two other questions concerning phase transitions in spin glasses in three dimensions: (i) is there a transition at finite temperature in isotropic vector spin glasses (such as Heisenberg), and (ii) is there a phase transition (AT line) in in a magnetic field in Ising spin glasses? By using Monte Carlo simulations, analyzed with finite-size scaling, I will argue that the answer to the first question is "yes", and to the second question is "no".

Phase transitions in complex networks

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The scale-free networks ($\gamma > 2$) which are randomised with fixed degree sequence are investigated. I introduce a model with exponential statistical weight of the form $\exp(\alpha T)$ assigned to each network where T is the number of triangles in the given network and α is an arbitrary parameter. The behaviour of thermalised system for different values of α is analysed. As a result, three phases with different topological and geometrical properties are distinguished: low triangle density phase (LT), high triangle density phase (HT) and saturated HT (SHT). Particularly, between the LT and HT the system undergoes first-order phase transition. The main characteristics of this phase transition are calculated with Metropolis and Wang-Landau algorithms. The transition between the HT and SHT has different nature and is defined by network breaking into many small components. In conclusion, a phase diagram for studied networks is presented.