Application of the density matrix renormalization group on Zq-symmetric models

Christophe Chatelain

Density Matrix Renormalization Group (DMRG) is an extremely powerful numerical tool for the determination of the ground state of 1-dimensional quantum chains or their 2-dimensional classical counterparts. We discuss a simple (and novel ?) method to improve stability by taking into account symmetries. We present preliminary results showing the cancellation of logarithmic terms in the calculation of amplitude ratios in the pure 4-state Potts model and a rough estimate of the phase diagram of the q-state clock model on a fully frustrated lattice.

A Monte Carlo study of the bond dilution in the Ising and Potts models in 3D

Pierre-Emmanuel Berche

The phase diagram of the bond diluted Ising and 4-state Potts models in 3D is investigated by Monte Carlo simulations. The 4-state Potts model undergoes a strong first-order phase transition in the pure case. The motivation of this work is then to characterize:
– the new stable disordered fixed point according to the Harris relevance criterion for the Ising model,
– the nature of the transition for the Potts model.

In the last case, for strong dilutions we obtain clear evidence for disorder induced second-order phase transition. The tricritical point, junction of the first and second order regimes along the dilution axis is numerically located and we give an estimation of the critical exponents in the second-order regime from a finite-size scaling study.

Quantum Monte Carlo studies of the anisotropic Heisenberg model

Jan Keller

A large class of d-dimensional quantum systems can be transformed to (d+1)-dimensional classical systems by the Trotter-Suzuki transformation. In a discrete extra dimension the anisotropic Heisenberg model transforms into a classical Ising model with four-spin interactions which can be simulated with a Monte Carlo algorithm. Cluster algorithms that elimininate critical slowing down can also be constructed. The basic procedures of the quantum Monte Carlo techniques are presented and further generalisations like continuous extra dimension, higher dimension or higher spins are touched.

Random field Ising model on the Bethe lattice

Thomas Nowotny

The phase diagram of the random field Ising model on the Bethe lattice with a symmetric dichotomous random field is investigated with respect to the transition between the ferromagnetic and paramagnetic regime. Refining arguments of Bleher, Ruiz and Zagrebnov [*J. Stat. Phys.* **93**, 33 (1998)] an exact upper bound for the existence of a unique paramagnetic phase is found which considerably improves the earlier results. Several numerical estimates of transition lines between a ferromagnetic and a paramagnetic regime are presented. The obtained results do not coincide with a lower bound for the onset of ferromagnetism proposed by Bruinsma [*Phys. Rev. B* **30**, 289 (1984)]. If the latter one proves correct this would hint to a region of coexistence of stable ferromagnetic phases and a stable paramagnetic phase. The talk is based on a joined work with Heiko Patzlaff and Ulrich Behn [*Phys. Rev. E* in print].

The gauge boson propagator of 3D compact electrodynamics in the confined and deconfined phases

Arwed Schiller

We investigate the gauge boson propagator in three dimensional compact Abelian gauge model in the Landau gauge at finite temperature. The monopole plasma leads to enhancement of the gauge boson propagator in the infrared region and to a depletion at $p^2 \approx 0$. The non-perturbative part of the propagator vanishes at the deconfinement transition caused by the monopoles pairing into dipoles. We discuss the relation between our results and the confining properties of the gluon propagator in gluodynamics which was under intense study recently.

Collective dynamics and fluctuations in a simple granular medium

Gudrun Schliecker

A simple realisation of a dense sheared granular medium is a closed chain of massive cylinders, located on a sliding horizontal plane and moving perpendicular to the cylinders' axes of rotation. The chain is confined by horizontal forces at both ends.

Whereas the perfect theoretical system is known to possess a steady state with well ordered collective rotational modes, its experimental realisation shows strong irregular oscillations of the rotation angles. The analysis of the experimental time series and theoretical simulations yield strong evidence that the observed dynamic fluctuations arise from temporally uncorrelated changes between different steady-state rotation patterns. In other words, the chain performs a collective random walk.

The jumps between different steady-state patterns can be traced to stress fluctuations arising from slight imperfections of the cylindrical shapes in the experiment. The 'noisy' dynamics appearing even in this simple, well ordered system underlines the generally observed high sensivity of dense granular materials to slight perturbations.

Universal scaling behaviour in the short-time regime of Monte Carlo simulations

Claudia Simoes

The short time dynamic approach is presented for two sophisticated versions of the Ising model on a square lattice.

Our simulations on (A) the Ising model with a line of defects reveal that the new critical exponent θ depends on the strength of the exchange coupling constant (J') of the altered line, while the dynamic critical exponent Z is not sensitive to it.

Our results for (B) the Ising model with three spin interactions confirm previous estimates for the static critical exponents β and ν. For the dynamic critical exponents Z and θ our results coincide with those of the 2D 4-state Potts model.

Simulating quantum dissipation in many-body systems

Ruggero Vaia

A path-integral Monte Carlo procedure is proposed to simulate the behavior of quantum many-body dissipative systems described within the framework of the Caldeira-Leggett influence functional. Thermodynamic observables are obtained by Monte Carlo sampling of the partition function after discretization and Fourier transformation in imaginary time of the dynamical variables. The method is tested for model systems, using realistic dissipative kernels. Results are also compared with the predictions of a recently proposed semiclassical approximation, thus testing the reliability of the latter approach for weak quantum coupling.

Effective temperature and pure-quantum renormalizations in the Heisenberg antiferromagnet on the square lattice

Paola Verrucchi

The field-theoretical result for the low-T asymptotic behavior of the correlation length of the Heisenberg antiferromagnet on the square lattice, as derived by the mapping onto the quantum nonlinear σ-model, has been recently improved by Hasenfratz (Eur. Phys. J. B**13**, 11 (2000)) in order to account for spins $S > 1/2$. We compare his expression with that obtained by the *pure-quantum self-consistent harmonic approximation* (PQSCHA) and show that the main outcome of the latter, i.e. that the quantum correlation length at a certain temperature t equals the classical one at a higher effective temperature defined in terms of the pure-quantum renormalization coefficients, remarkably holds also when the field-theoretical approach is adopted. Such result allows us to draw a general picture of the thermodynamics of the system, in which both semiclassical and field-theoretical results consistently find their own range of validity.

Despite not being the direct outcome of a numerical work, this result comes as an answer to the many questions posed by the most recent quantum Monte Carlo data on the 2dQHAF, whose analysis has actually inspired the work itself.

Computer simulation techniques for dense molecular and inhomogeneous fluids: Extended ensembles and virtual parameter variation

Horst-Ludger Vörtler
(horst.voertler@physik.uni-leipzig.de)

A basic problem in the simulation of chemical potentials and phase equilibria of fluids at high density and/or geometric restrictions is the very low probability of test particle insertion on those conditions. This restricts the applicability of standard techniques as Widoms test particle method or Gibbs Ensemble approach.

To address this problem gradual particle insertion techniques [1] are discussed which facilitate the transition from a N-particle to a $N+1$-particle system by passing through a chain of canonical ensembles with a scaled particle. The implementation of this technique to the estimation of chemical potentials of associating fluids will be presented.

Combining gradual particle insertion with the Gibbs Ensemble technique a chain of Gibbs Ensembles (Extended Gibbs Ensemble) is obtained which allows the simulation of phase equilibria of fluids consisting of highly non-spherical molecules (Kihara fluids) [2] on conditions where conventional methods fail.

A novel technique for the direct simulation of partition function derivatives of (inhomogeneous) fluids by means of virtual parameter variation will be presented too [3]. Varying the number of particles by virtual particle insertion Widom's method is recovered. Virtual volume variation offers an alternative route for pressure calculations in complex fluids, particularly, allowing the estimation of 'thermodynamic' pressures in inhomogeneous systems.

[1] Nezbeda, I.; Kolafa, J.; Molec. Simulation **5** (1991) 391., Kolafa, J.; Vörtler, H.L.; Aim, K.; Nezbeda, I.; Molec. Simulation **11** (1993) 5.

[2] Kettler, M.; Vörtler, H.L.; Nezbeda, I.; Strnad, M; Fluid Phase Equilibria **181** (2001) 83.

[3] Vörtler, H.L.; Smith, W.R.; J. Chem. Phys. **112** (2000) 5168.

Vertex models on dynamical quadrangulations

Martin Weigel

We consider the coupling of ice-type vertex models to random, planar ϕ^4 quantum-gravity graphs. The well-established techniques for the simulation of dynamical triangulations and their dual ϕ^3 graphs are suitably adapted to the case of four-valent graphs. These methods are combined with a formulation of the *loop algorithm* for the simulation of the vertex model matter part. We present a preliminary analysis of the dynamical scaling behaviour of the combined algorithm for the case of the 6-vertex model coupled to quantum gravity.

Monte Carlo simulations of critical dynamics far from equilibrium

Bo Zheng

With Monte Carlo methods we have systematically studied the short-time behaviour of critical dynamics. The new critical exponent θ is determined. Based on the scaling form in short-time critical dynamics, new methods for determining the critical temperature and all the static exponents as well as the dynamic exponents have been proposed. These methods do not suffer from critical slowing down. General applications are attractive. Furthermore, short-time dynamic scaling behavior has been found also in dynamic systems described by microscopic deterministic equations of motion. Fundamental problems in statistical physics are touched.