ABSTRACTS

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Visualization of atomistic simulations

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Monte Carlo and Molecular Dynamics simulations made in the Computational Physics Group at the Technion will be described. These include modeling of diamond/graphite systems and aluminium/alumina interfaces, as well as studying defects in copper and vanadium. Examples of new physics results obtained thru our visualizations of simulation samples will be given. I will introduce the AViz package my group has developed which facilitates discussion with experimental collaborators and presentation. Early steps in the application of AViz to spin systems will also be described.

Generalized-ensemble simulations of off-lattice heteropolymers

Michael Bachmann

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First results of the application of a multicanonical algorithm to a modified AB model, which is an effective off-lattice model for heteropolymers, are presented. In this simplified model, heteropolymers are considered as chains of hydrophobic (A) and hydrophilic (B) monomers only. Into the energy function enter the bending energy and a Lennard-Jones-like potential between nonbonded monomers, where short-range repulsion and long-range attraction compete. Contacts between hydrophobic monomers are favoured, thereby assuming that the global energy minimum state of proteins is characterized by a compact hydrophobic core screened from the solvent by a shell of hydrophilic residues. We calculate thermodynamic quantities and identify temperatures, where conformational pseudo transitions are expected. Since the multicanonical algorithm allows for an accurate sampling of the low-temperature region, we also obtain good estimates for the global energy minimum.

Critical behaviour of non-equilibrium phase transitions

Ulrich Behn

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We describe non-equilibrium phase transitions in arrays of dynamical systems with cubic nonlinearity driven by multiplicative Gaussian white noise. We discuss the phase diagram, the order of the transitions, and the critical behaviour. For global coupling we show analytically that the critical exponent of the order parameter exhibits a transition from the value 1/2 to a non-universal behaviour depending on the ratio of noise strength to the magnitude of the spatial coupling.

Monte Carlo simulations of the 3D bond-diluted 4-state Potts model

Bertrand Berche

LPM, Université Henri Poincaré, Nancy, France

Large-scale Monte Carlo simulations of the bond-diluted three-dimensional 4-state Potts model are performed. The phase diagram and the physical properties at the phase transition are studied using finite-size scaling techniques. Evidences are given for the existence of a tricritical point dividing a regime where the transition remains of first order and a second regime where the transition is softened to a continuous one by the influence of disorder. In the former regime, the nature of the transition is essentially clarified through an analysis of the energy probability distribution. In the latter regime critical exponents are estimated. Rare and typical events are identified and their role is qualitatively discussed in both regimes.

Phase structure of a generalized ψ^4 model

Elmar Bittner

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Using Monte Carlo simulations, we analyze the critical behaviour of the Ginzburg-Landau model in the presence of an additional fugacity term. With this modification we can show that the complex $|\psi|^4$ theory can be tuned to undergo a first-order transition by varying the strength of the new term in the generalized Hamiltonian. From a finite-size scaling analysis we determine the critical endpoint of the line of first-order phase transitions for several values of the strength of the new term in the generalized Hamiltonian. Based on these results we sketch the phase diagram of the generalized complex $|\psi|^4$ model.

Simulations of star polymers: Scaling of single stars and star-star effective interaction potentials

Peter Grassberger

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We present large statistics simulations of 3-dimensional star polymers with up to $f = 80$ arms, and with up to 4000 monomers per arm for small values of f. They were done for the soft-exclusion Domb-Joyce model on the simple cubic lattice. Due to the finite monomer-monomer repulsion, we can attach an arbitrary number of arms to a single central site. This, together with using the 'magic' value for the repulsion strength, minimizes corrections to scaling. Using the PERM chain growth algorithm (modified to allow simultaneous growth of all arms), we can measure not only the swelling (as observed from gyration radii and center-to-end distances), but also the partition sum. The latter gives very precise estimates of the critical exponents γ_f. We also study the effective pair potential between two star polymers with equal arm lengths and equal number f of arms. We find that this potential is much less soft than claimed in previous papers, in particular for $f \gg 1$. We verify the logarithmic divergence of $V(r)$ for $r \to 0$, with r being the distance between the two cores, predicted by Witten and Pincus. But we find for $f > 20$ that the Mayer function is practically indistinguishable from that for a Gaussian potential.

Critical exponents and universal amplitude ratios from improved models

Martin Hasenbusch

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We study improved models in the Ising, XY and Heisenberg universality classes using Monte Carlo simulations and high-temperature series expansions. Among other models, we consider the ϕ^4 model on the lattice. Using a finite size scaling method, the value λ^* of the parameter in the potential term is determined, where leading confluent corrections vanish. Based on this result, we obtain most accurate estimates for the critical exponents and for a number of universal amplitude ratios.

Simulations of Met-Enkephalin with solvent-accessible area parameterizations

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We investigate the solvent-accessible area method by means of Metropolis simulations of the brain peptide Met-Enkephalin at $300\,K$. For the energy function ECEPP/2 nine atomic solvation parameter (ASP) sets are studied that had been proposed by previous authors. The simulations are compared with one another, with simulations with a distance dependent electrostatic permittivity $\epsilon(r)$, and with vacuum simulations ($\epsilon = 2$). Parallel tempering and the biased Metropolis techniques RM_1 are employed and their performances are evaluated. The measured observables include energy and dihedral probability densities (pds), integrated autocorrelation times, and acceptance rates. Two of the ASP sets turn out to be unsuitable for these simulations. For all other systems selected configurations are minimized in search of the global energy minima, which are found uniquely for the vacuum and the $\epsilon(r)$ system, but not for any of the ASP models. Other observables show a remarkable dependence on the ASPs. In particular, three ASP sets have much smaller autocorrelations at 300 K than the vacuum simulations, opening the possibility that simulations can be speeded up vastly by judiciously choosing details for the force field.

Off-equilibrium dynamics in 2D XY model: Two-time functions

Dragi Karevski

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We study the non-equilibrium time evolution of the classical XY spin model in two dimensions. The two-time autocorrelation and linear response functions are considered for systems initially prepared in a high-temperature state and in a completely ordered state. After a quench into the critical phase, we determine, via Monte Carlo simulations, the time-evolution of these quantities and extract the temperature dependence of the slope of the parametric plot susceptibility/correlation in the asymptotic regime. This slope is usually identified with the infinite fluctuation-dissipation ratio which measures the violation of the equilibrium fluctuation-dissipation theorem. However, a direct measure of this ratio leads to a vanishing value.

Phase transitions in the asymmetric exclusion process

Ralph Kenna

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The 1D Asymmetric Exclusion Process (ASEP) is a paradigm for non-equilibrium dynamics, in particular driven diffusive processes. It is usually considered in a canonical ensemble in which the number of sites is fixed. We observe that the *grand*-canonical generating function for the ASEP is remarkably simple, and use it to discuss the Lee-Yang zeros of the steady-state normalization, which plays the role of the partition function of equilibrium systems.

Random-matrix theory as a discriminator between quantum chaos and regularity in ϕ^4 theory

Harald Markum

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We are checking the eigenvalue spectrum of the Φ^4_{1+1} Hamiltonian against Poisson or Wigner behavior predicted from random-matrix theory and present some preliminary results. More generally, we discuss random matrix theory as a tool to discriminate the validity of a model Hamiltonian compared to the underlying theory or experimental data.

Transport phenomena in mesoscopic systems simulated within a thermodynamic framework

Harald Morgner

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Standard thermodynamics does not employ in general a spatial coordinate. Thus, the treatment of interfaces with a strong gradient of density or composition is usually outside the range of this theory. The formulation given by Cahn and Hilliard for the description of interfaces is useful, but limited to equilibrium. The Cahn-Hilliard theory [1] can be shown to suffer from the fact that it gets conceptually wrong in non-equilibrium situations. Some time ago, I have derived a definition of the chemical potential for the general case, i.e. for all situations including those with strongly varying density and/or composition and irrespective of a proximity to equilibrium. On this basis, the Onsager ansatz for diffusion allows to propagate in time any given distribution of matter under the gradient of the chemical potential as driving force. More recently, I have found that this generalized definition of the chemical potential yields as well the basis to explore the range of validity of the Navier-Stokes equation. It turns out that the pressure gradient as driving force has to be replaced by a quantity containing the gradient of the chemical potential. This new expression for the driving force of convection develops into the pressure gradient in homogeneous environment but deviates significantly from it in inhomogeneous environment, e.g. at interfaces. As this statement holds not only for fluid/fluid interfaces, but as well for fluid/solid interfaces it appears likely that this finding has some bearing on the topic of nanofluidics.

[1] J.W. Cahn and J.E. Hilliard, J. Chem. Phys. **28**, 258 – 267 (1958).

A study of 3D dual superconductivity

Thomas Neuhaus

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We show that fluctuating 3D Ginzburg Landau theory reduces to classical 3D XY theory for coupling parameters in the type II superconducting region at the critical point.

Ising droplets in action

Andreas Nußbaumer

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The multimagnetic algorithm simulates an artifical ensemble where every value of the magnetisation has the same probability. Still, simulations of simple models show barriers in the magnetisation that scale with the inverse temperature β and the system size L. Making use of analytic work by Leung and Zia [1], Neuhaus and Hager [2] recently explained this behaviour in the case of the two-dimensional Ising model with the occurrence of a geometrically induced first-order transition from a droplet to a strip domain. Using Fourier coefficients to define the geometric anisotropy of a configuration a comparison with an analytical description of the transition behaviour (deformation of a droplet into a stripe) was possible. From the scaling of the anisotropy for different system sizes when simulated with Kawasaki dynamics (M = const.) a value for the barrier size was obtained. For the three-dimensional case a set of new transitions could be identified and the crystal shapes during the transitions were measured.

[1] K. Leung and R. Zia, Geometrically induced transitions between equilibrium crystal shapes, J. Phys. A **23**, 4593 (1990).
[2] T. Neuhaus and J. Hager, 2D crystal shapes, droplet condensation, and exponential slowing down in simulations of first-order phase transitions, Stat. Phys. **113**, 47 (2003).

Ageing phenomena in ferromagnets

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Ageing phenomena are observed in a broad variety of systems with slow relaxation dynamics. Useful insight may often be gained via the consideration of simple ferromagnetic models (rather than genuinely glassy systems), quenched from a disordered initial state into the low-temperature phase. For their study two-time quantities, like correlation and response functions, are particularly useful. These quantities display dynamical self-similarity in the ageing regime. In this talk I will discuss the recent progress achieved in the study of ageing phenomena in ferromagnets. I will show that exact expressions for response functions can be obtained from the theory of local scale invariance. These expressions will be tested in kinetic Glauber-Ising models.

Physics in geometrical Potts clusters

Adriaan Schakel

Institut für Theoretische Physik, FU Berlin, Germany

The critical properties of the two-dimensional Potts models are encoded in the fractal structure of the Fortuin-Kasteleyn clusters of like spins. These clusters, better known to the Monte-Carlo community as Swendsen-Wang clusters, derive from the naive geometrical clusters. In this talk, it is shown that (i) the fractal structures of the two cluster types are in one-to-one correspondence and that (ii) the geometrical clusters also encode critical behavior, namely that of the tricritical fixed point of the diluted Potts model. To support these results, a novel Monte Carlo study is presented in which the high-temperature representation of the 2-state Potts (Ising) model is simulated by means of a plaquette update.

Perturbative renormalization of bilinear quark operators

Arwed Schiller

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One-loop lattice renormalisation factors of bilinear quark operators are calculated using overlap fermions and improved gauge actions including six-link loops. We show how to apply tadpole improvement to overlap fermions. An analytic proof is given that the gauge dependent parts of the quark self energy and the Green functions are indepedent of the lattice fermion representation.

Universal energy distribution for interfaces in a random field environment

Semjon Stepanow

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We study the energy distribution function $\rho(E)$ for interfaces in a random field environment at zero temperature by summing the leading terms in the perturbation expansion of $\rho(E)$ in powers of the disorder strength, and by taking into account the non perturbational effects of the disorder using the functional renormalization group. We have found that the average and the variance of the energy for one-dimensional interface of length L behave as, $\langle E\rangle \sim L \ln L$, $\Delta E \sim L$, while the distribution function of the energy tends for large L to the Gumbel distribution of the extreme value statistics.

Ising model with kinetical restrictions

Steffen Trimper

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We consider the kinetical Ising model with self-organized restrictions to mimic the cooperativity inherent in glasses and undercooled liquids. The inclusion of restrictions leads to significant slowing down of the relaxation time and to a stretched exponential decay of the autocorrelation-function. The model can be studied with analytical methods based on a Master-equation in a Fock-space representation and by Monte Carlo simulations.

MC simulation of associating fluids: Chemical potentials, phase equilibria, and critical properties

Horst L. Vörtler

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We discuss recent Monte Carlo computer simulation techniques to calculate efficiently chemical potentials of short-ranged primitive models of associating (water-like) fluids, where the conventional Widom test-particle method fails because of the very low insertion probability of a test particle at moderate to high densities. Therefore, gradual particle insertion and monomer insertion techniques are used to overcome these problems. We present novel simulation results for chemical potential versus density isotherms of primitive water models which show typical van derWaals loops at sub-critical temperatures. We use these data to estimate the densities of the coexisting fluid phases by means of a Maxwell equal-area construction. From the vapour-liquid equilibrium data we calculate the critical temperatures and the critical densities of primitive water using classical scaling theory arguments. The presented chemical potentials and coexistence properties should be considered as important reference data for molecular-based perturbation theories of associating fluids.