DY 1: Critical phenomena and phase transitions

Time: Monday 10:00–12:00 Location: MA 004

Invited Talk DY 1.1 Mon 10:00 MA 004

The Thermodynamic Casimir Effect: Monte Carlo Results — •Alfred Hucht — Theoretische Physik, Universität Duisburg-Essen, 47048 Duisburg

The thermodynamic Casimir effect describes a force between the boundaries of thin films mediated through long-range fluctuations of the order parameter near a continuous phase transition. This force is universal for a given universality class and boundary condition, and can be attractive or repulsive.

The universal finite size scaling function of the critical Casimir force for the three dimensional XY and Ising universality class with different boundary conditions is determined using Monte Carlo simulations [1]. The results are in excellent agreement with recent experiments on ^{4}He Films at the superfluid transition [2] and with experiments on binary liquid mixtures [3].

[1] A. Hucht, Phys. Rev. Lett. 99, 185301 (2007).
[2] R. Garcia and M. H. W. Chan, Phys. Rev. Lett. 83, 1187 (1999).
[3] M. Fukuto *et al.*, Phys. Rev. Lett. 94, 135702 (2005).

DY 1.2 Mon 10:30 MA 004

Autocorrelation times and the parallel tempering algorithm — •Elmar Bittner, Andreas Nussbaumer, and Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

We introduce a new update schema for systematically improving the efficiency of parallel tempering Monte Carlo simulations by taking the temperature dependence of autocorrelation times into account. In contrast to previous attempts the temperature is fixed and chosen in such a way that the acceptance rate for all adjacent replica is about 50%. We show that by adopting the numbers of local updates between the parallel tempering moves, the round-trip times of a replica between the lowest and the highest temperatures is significantly increased, and therefore, the efficiency of the parallel tempering algorithm is considerably improved. As examples we show results for the two-dimensional Ising model and the three-dimensional Edwards-Anderson spin glass.

DY 1.3 Mon 10:45 MA 004

Spin-1/2 XX chain with three-site interactions: Dynamic properties — •Joachim Stolze[1], Oleg Derzhko[2], Taras Krokhmalskii[2], and Taras Verkholyak[2] — [1]Institut für Physik, TU Dortmund, Germany — [2]Institute for Condensed Matter Physics, L'viv, Ukraine

We consider a spin-1/2 XX chain in a transverse (z) field with (XZX+YZY)-type three-site interactions. After performing the Jordan-Wigner transformation to spinless fermions, these interactions induce only a (real) next-nearest-neighbor hopping of spinless fermions preserving the exact solvability of the problem. We focus on dynamic properties of the model in its various ground-state phases. We report a closed-form expression for the zz dynamic structure factor and for some other dynamic structure factors all of which are governed by a two-fermion (particle-hole) excitation continuum. We examine the properties of the two-fermion excitation continuum (boundaries, soft modes, van Hove singularities). The xx dynamic structure factor is governed by many-fermion excitations. We report both analytical (in the high-temperature limit and in the zero-temperature strong-field regime) and numerical results for this dynamic structure factor. Throughout our study we discuss in some detail those features of the dynamic structure factors which indicate the presence of the three-site interactions.

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DY 1.4 Mon 11:00 MA 004

Negative-weight percolation — •Oliver Melchert and Alexander K. Hartmann — Institut für Physik, Universität Oldenburg, 26111 Oldenburg

We describe a percolation problem on lattices, with edge weights drawn from disorder distributions that allow for weights of either sign, i.e. including negative weights. We are interested whether there are spanning paths or loops of total negative weight. This kind of percolation problem is fundamentally different from conventional percolation problems, e.g. it does not exhibit transitivity, hence no simple definition of clusters, and several spanning paths/loops might coexist in the percolation regime at the same time. To study this percolation problem numerically, one has to perform a non-trivial transformation of the original graph and apply sophisticated matching algorithms.

Here, we study the corresponding percolation transitions on large square and cubic lattices for two types of disorder distributions and determine the critical exponents. The results show that negative-weight percolation is in a different universality class compared to conventional bond/site percolation. On the other hand, negative-weight percolation seems to be related to the ferromagnet/spin-glass transition of random-bond Ising systems, at least in two dimensions.

DY 1.5 Mon 11:15 MA 004

Multifractality of self-avoiding random walks on percolation cluster — •Viktoriya Blavatska[1,2] and Wolfhard Janke[2] — [1]Institute for Condensed Matter Physics of the National Academy of Sciences of Ukraine, Lviv, Ukraine — [2]Institut für Theoretische Physik, Universität Leipzig, Leipzig, Germany

The model of self-avoiding walks (SAWs) on disordered lattice perfectly describes the universal properties of long flexible polymer chains in porous media. In our study, disordered lattice is exactly at the percolation threshold. Applying the pruned-enriched Rosenbluth chain-growth method (PERM), we perform numerical simulations of SAWs on the backbone of the incipient percolation cluster in two, three and four dimensions. Considering higher order correlations of SAWs, we study the multifractal properties of the model. Our results bring about the estimates of critical exponents, governing the scaling laws of configurational properties of SAWs.

DY 1.6 Mon 11:30 MA 004

Molecular Dynamics simulations of the phase separation of polymer solutions in thin film geometry — •Katarzyna Bucior, Leonid Yelash, and Kurt Binder — Institute of Physics, Johannes-Gutenberg University of Mainz, Mainz, Germany

We use a coarse-grained model of hexadecane dissolved in supercritical carbon dioxide to simulate the phase separation, initiated by quenching a system into an unstable region of the phase diagram, e.g. by temperature or pressure jumps. The parameters of the model are fitted to reproduce critical parameters of hexadecane and carbon dioxide. The study is performed in slit like pores, formed by two infinite parallel walls consisting of spherical particles.

We present the typical results for the observed time evolutions during phase separation for this model, structure factors, snapshot pictures, density profiles, density distributions. Since the behavior of the system depends on the distance from the wall, we calculate some properties in layers parallel to the walls. The time dependence of the characteristic domain size is also discussed.

DY 1.7 Mon 11:45 MA 004

Investigation of adsorption of star polymers in the framework of massive field theory approach — •Zoryana Usatenko — Leibniz Institute for Polymer Research Dresden e.V., 01069 Dresden, Germany — Institute for Condensed Matter Physics, NAS Ukraine, 79011 Lviv, Ukraine

Adsorption on a planar repulsive and "inert" wall of a star polymer with f arms with the same length immersed in a good solvent are studied on the basis of renormalization group field theoretical approach directly in d=3 dimensions for one-loop order. The performed scaling analysis is based on formal analogy between the polymer adsorption problem and the equivalent problem of critical phenomena in the semi-infinite n-vector model (in the limit $n \to 0$) with a planar boundary. The case of a center adsorbed star and star polymer with two adsorbed arm ends are considered. We have calculated the configuration-number exponents $\gamma(f)$ for center adsorbed star and $\gamma_{II}(f)$ for two ends adsorbed star polymer. The obtained results for critical exponents are compared with results obtained in the framework of ϵ - expansions. We also calculated the mean force between free star polymer and surface.