DY 31: Phase Transitions and Critical Phenomena

Time: Friday 9:30–13:30 Location: MA 004

Topical Talk DY 31.1 Fri 9:30 MA 004

Pair Superfluidity of Constrained Bosons in Two Dimensions — •Stefan Wessel[1] and Lars Bonnes[2] — [1]RWTH Aachen University, Germany — [2]University of Innsbruck, Austria

Bose gases with attractive interactions can form two different superfluid phases. Besides the conventional (atomic) superfluid, a molecular superfluid of boson pairs can form, with exhibits half-vortex topological defects. To prevent the attractive Bose gas from collapse, a scenario has been recently been proposed, where the particles are constrained to an optical lattice and furthermore subject to strong three-body losses, that project out triple occupancy on each lattice site. Employing quantum Monte Carlo simulations, we study the quantum phase transition between these atomic and dimer superfluids. Evidence is provided for the existence of a tricritical point along the saturation transition line, where the transition changes from being first-order to a continuous transition of the dilute bose gas of holes. We show that the thermal disintegration of the pair superfluidity is governed by the proliferation of fractional half-vortices leading to an Berezinskii-Kosterlitz-Thousless transition with an anomalous stiffness jump. In addition to the (conventional) Berezinskii-Kosterlitz-Thousless transition out of the atomic superfluid, we furthermore identify a direct thermal phase transition separating the pair and the atomic superfluid phases, and show that this transition is continuous with critical scaling exponents consistent with those of the two-dimensional Ising universality class.

DY 31.2 Fri 10:00 MA 004

Loop percolation — •Matthias J. F. Hoffmann, Susan Nachtrab, Gerd E. Schröder-Turk, and Klaus Mecke — Institut für Theoretische Physik, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

We report a new planar percolation model, called *loop percolation*, which is in a different universality class than the conventional bond- or site percolation models. The model is defined by randomly disconnecting, with probability p, the degree-four nodes of a planar square lattice into two unconnected degree-two nodes; for each disconnection, the two possible orientations are chosen randomly with the probability $x = 1/2$. The extremal configurations are the periodic square lattice (at $p = 0$ with no disconnected nodes) and a configuration of many self-avoiding unbranched random walks, "spaghetti state", when all nodes are disconnected at $p = 1$. Numerical analysis shows that this model has a percolation transition at $p_c = 1$, that is, only when all nodes are disconnected. The critical exponents ($\beta = 1/3$, $\nu = 4/3$, $\gamma = 67/36$, $D_f = 79/48$) of this transition are numerically shown to be significantly different from those of the conventional bond- or site-percolation model, and to agree with a mapping to the six-vertex model. Further, when suitably generalized to $x \neq 1/2$ the model shows a percolation transition at $p_c = (1 + |2x - 1|)^{-1}$ with the critical bond/site percolation exponents for all $x \neq 1/2$.

DY 31.3 Fri 10:15 MA 004

Mean-field behavior of the negative-weight percolation model on random regular graphs — •Oliver Melchert[1], Alexander K. Hartmann[1], and Marc Mezard[2] — [1]Institut für Physik, Universität Oldenburg (Germany) — [2]Laboratoire de Physique Théorique et Modeles Statistiques, Université de Paris Sud (France)

In the presented study, we investigate the critical properties of minimum-weight loops and paths in the negative-weight percolation (NWP) problem on 3-regular random graphs (RRGs), i.e. graphs where each node has exactly 3 neighbors and were there is no regular lattice structure [1]. By studying a particular model on RRGs, one has direct access to the mean-field exponents that govern the model for $d > d_u$. The presented study aims to support the previous conjecture $d_u = 6$ [2] by directly computing the mean field exponents for the NWP model with a bimodal weight distribution, and comparing them to those found for a regular hypercubic lattice with dimension $d = 6$. The presented results are obtained via computer simulations, using an appropriate mapping to a matching problem, as well as by analytic means, using the replica symmetric cavity method for a related polymer problem. We find that the numerical values for the critical exponents on RRGs agree with those found for $d = 6$-dimensional hypercubic lattice graphs within errorbars and hence support the conjectured upper critical dimension $d_u = 6$.

[1] OM, A.K. Hartmann, and M. Mézard, PRE 84, 041106 (2011)
[2] OM, L. Apolo, and A.K. Hartmann, PRE 81, 051108 (2010)

DY 31.4 Fri 10:30 MA 004

The two-dimensional Ising spin glass at zero temperature — •Hamid Khoshbakht[1], Martin Weigel[1,2], and Jacob D. Stevenson[3] — [1]Institut für Physik, Johannes Gutenberg-Universitaät Mainz, D-55099 Minz, Germany — [2]Applied Mathematics Research Center, Coventry University, Coventry, CV1 5FB, UK — [3]University Chemical Laboratories, Lensfield Road, Cambridge, CB2 1EW, UK

Ground states for the Ising spin glass in two dimensions can be determined in polynomial time as long as periodic boundary conditions are applied at most in one direction. Using a recently proposed mapping to an auxiliary graph decorated with Kasteleyn cities, we determine ground states for systems with open-periodic boundary conditions for lattices of linear sizes up to $L = 9000$ and calculate defect energies as well as domain-wall lengths. Although the matching approach does not work for periodic-periodic boundaries, where less finite-size corrections are expected, using a windowing technique allows to determine quasi-exact ground-states for lattices up to $L = 3000$. By using these techniques, we arrive at high-precision estimates of the spin-stiffness exponent and the domain-wall fractal dimension for Gaussian as well as bimodal couplings. We compare the geometry of the thus generated domain walls with the detailed predictions given for random curves in the plane in the framework of Schramm-Loewner Evolution (SLE).

DY 31.5 Fri 10:45 MA 004

One-dimensional Vector Spin Glasses with Long-Range interactions — •Frank Beyer[1] and Martin Weigel[1,2] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55099 Mainz, Germany — [2]Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, England

One-dimensional spin-glass models with power-law interactions allow for numerically tackling large linear system sizes. At the same time tuning the interaction range enables to study systems with zero-temperature transitions, with non-trivial finite-temperature transitions and in the mean-field regime, respectively. Here, we focus on the case of vector spin glasses with an infinite number of spin components which shows some important differences as compared to models with a finite number of components. Using extensive numerical calculations at zero and finite temperatures, we determine the phase diagram of the model and elucidate its critical behavior in the mentioned regimes.

DY 31.6 Fri 11:00 MA 004

Isotropic-polar phase transitions in an amphiphilic fluid — Michael Melle[1], Stefano Giura[1], Sergej Schlotthauer[1], and •Martin Schoen[1,2] — [1]Stranski-Lab. f. Physikalische und Theoretische Chemie, Technische Universität Berlin, Straße des 17. Juni 115, 10623 Berlin, Germany — [2]Dept. of Chemical and Biomolecular Engineering, North Carolina State University, 911 Partners Way, Raleigh, NC 27695, USA

We present Monte Carlo simulations of the isotropic-polar (IP) phase transition in an amphiphilic fluid carried out in the isothermal-isobaric ensemble. Our model consists of Lennard-Jones spheres where the attractive part of the potential is modified by an orientation-dependent function. This function gives rise to an angle dependence of the intermolecular attractions corresponding to that characteristic of point dipoles. Our data show a substantial system-size dependence of the dipolar order parameter. We analyze the system-size dependence in terms of the order-parameter distribution and a cumulant involving its first and second moments. The order parameter, its distribution, and susceptibility observe the scaling behavior characteristic of the 3D-Ising universality class. Because of this scaling behavior and because all cumulants have a common intersection irrespective of system size we conclude that the IP phase transition is continuous. Considering pressures $1.3 \leq P \leq 3.0$ we demonstrate that a line of continuous phase transition exists which is analogous to the Curie line in systems exhibiting a ferroelectric transition. Our results are qualitatively consistent with Landau's theory of continuous phase transitions.

DY 31.7 Fri 11:15 MA 004

Dynamical quantum phase transitions for quenches in the transverse field Ising model — •Markus Heyl[1], Anatoli Polkovnikov[2], and Stefan Kehrein[1] — [1]Department of Physics, Arnold Sommerfeld Center for Theoretical Physics, Ludwig-Maximilians-Universität München — [2]Department of Physics, Boston University

We study quenches of the magnetic field in the transverse field Ising model. For quenches across the quantum critical point, the boundary partition function in the complex temperature-time-plane shows lines of Fisher zeros that intersect the time axis, indicating non-analytic real-time evolution in the thermodynamic limit (analogous to well-known thermodynamic phase transitions). We characterize these dynamical quantum phase transitions through topological quantum numbers and show that the dynamic behavior generates a new emergent non-equilibrium energy scale. We argue that this behavior is expected to be generic for interaction quenches across quantum critical points in other models as well.

15 min. break

DY 31.8 Fri 11:45 MA 004

Properties of stable and metastable crystals and interfaces in the hard sphere system — •Mohammad Hossein Yamani and Martin Oettel — Institute of Physics, Johannes Gutenberg University, Mainz, Germany

Colloidal hard spheres are an intensely studied model system for addressing the nucleation problem. Understanding homogeneous and heterogeneous nucleation requires a precise knowledge about equilibrium crystal structures, crystal-liquid surface tensions and interface tensions with substrates. Density Functional Theory (DFT) as one of the core theoretical approaches of statistical physics of fluids and crystals, is able to treat such an important system successfully and accurately. We use density functional theory of fundamental measure type (FMT) to obtain the fully minimized periodic FCC crystal profiles and wall-liquid interface tensions and compare to new, accurate simulation data. Furthermore we present first DFT results obtained by unconstrained minimization for free energies of metastable BCC and HCP crystals. DFT results in the case of FCC compare very well to simulation results. HCP and FCC differ only in the stacking sequence of hexagonally packed planes of particles, and thus one expects only a small free-energy difference between these two structures. We present preliminary results obtained by FMT for the differences between FCC and HCP in free-energy and in the unit cell density distribution.

DY 31.9 Fri 12:00 MA 004

On phase-field modeling with a highly anisotropic interfacial energy — •Michael Fleck, Leslie Mushongera, Denis Pilipenko, Kumar Ankit, and Heike Emmerich — Materials and Process Simulation, University of Bayreuth, Germany

The crystalline nature of solids results in the anisotropy of many thermophysical parameters. In particular, the interfacial energy between different phases is often found to be a function of the crystallographic orientation of the interface. We report on phase-field approaches that allow for anisotropies sufficiently high so that the interface develops facets as well as sharp corners due to missing crystallographic orientations. The latter implies the necessity of a regularization that enforces local equilibrium at the corners, to remove the ill-posednes of the phase field evolution equation. Two different anisotropic phase-field formulations are presented and discussed: The classical model that allows the interface to vary with orientation, and another more recent formulation that has a constant interface width. Further, we develop an explicit finite difference scheme that combines a two-step differentiation with a stagnation grid formulation. The presented numerical implementation is stable and accurate enough to account for odd crystal symmetries and high angle rotations of the initial crystalline orientation. Even in the case of highly anisotropic interfacial energies, both formulations show excellent agreement with the well-known Wulff construction of the equilibrium shape of a particle embedded in a matrix.

DY 31.10 Fri 12:15 MA 004

Improved Linear Programming applied to the Vertex Cover Problem — •Timo Dewenter and Alexander K. Hartmann — Institut für Physik, Universität Oldenburg, 26111 Oldenburg

We consider the well studied [1] NP-complete Vertex Cover problem (VC) on Erdős-Rényi (ER) random graphs with finite connectivity c.

Previously, we applied the mapping of VC to a Linear Programming problem (LP), where the nodes of the graph are represented by real-valued variables $x_i \in [0,1]$. A value of $x_i = 0$ means that the node is uncovered and $x_i = 1$ denotes a covered node. Each edge $\{j,k\}$ in the graph is related to a constraint $x_j + x_k \geq 1$ in the LP. The Simplex-algorithm is then applied to solve this LP, but for larger c incomplete solutions with variables $x_i \in]0,1[$ are found. So we used a cutting-plane approach that adds constraints to the LP based on loops in the graph with odd length leading typically to exact solutions for $c < e \approx 2.718$.

Here, we solve small subgraphs $G_S = (U, E_U)$ with an exact algorithm and add contraints $\sum_{x_i \in U} \geq |V_C(G_S)|$ to the LP, where $|V_C(G_S)|$ is the size of the minimum VC of G_S. This leads in principle to complete solutions, but here we only use $|U| \leq 10$. The behaviour of this algorithm is studied for ER random graphs as a function of c. After performing statistical analyses [2] for different system sizes, we compare with the phase diagram for the critical fraction x_c of covered vertices.

[1] M. Weigt and A.K. Hartmann, Phys. Rev. Lett. **84**, 26 (2000)
[2] A.K. Hartmann: *Practical Guide to Computer Simulations*, World-Scientific, 2009

DY 31.11 Fri 12:30 MA 004

Simulation of critical phenomena in fluids with the Lattice Boltzmann method — •Markus Gross and Fathollah Varnik — ICAMS, Ruhr-Universität Bochum, Germany

Recently, thermal fluctuations have been introduced into the Lattice Boltzmann method for non-ideal fluids, allowing one to numerically solve the fluctuating Navier-Stokes equations for an isothermal liquid-vapor system. Here, it is demonstrated that the method, employing a Ginzburg-Landau free energy functional, correctly reproduces the static critical behavior associated with the Ising universality class. A particular focus will be on finite-size effects and issues related to the global conservation of the order-parameter. Additionally, the critical behavior of the transport coefficients (speed of sound, shear and bulk viscosity) of the model, which describes an isothermal compressible fluid, is discussed.

DY 31.12 Fri 12:45 MA 004

Numerical study of polymer adsorption on a fractal substrate — Viktoria Blavatska[1,2] and •Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Germany — [2]Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, Lviv, Ukraine

We study the adsorption of flexible polymer macromolecules on a percolation cluster, formed by a regular two-dimensional disordered lattice at critical concentration p_c of attractive sites. The percolation cluster is characterized by a fractal dimension $d_s^{p_c} = 91/49$. The conformational properties of polymer chains grafted to such a fractal substrate are studied by means of the pruned-enriched Rosenbluth method (PERM). We find estimates for the surface crossover exponent governing the scaling of the adsorption energy in the vicinity of the transition point, $\phi_s^{p_c} = 0.425 \pm 0.009$, and for the adsorption transition temperature, $T_A^{p_c} = 2.64 \pm 0.02$. As expected, the adsorption is diminished when the fractal dimension of the substrate is smaller than that of a plain Euclidean surface. The universal size and shape characteristics of a typical spatial conformation which attains a polymer chain in the adsorbed state are analyzed as well.

Topical Talk DY 31.13 Fri 13:00 MA 004

Multifractal fluctuations and Scaling at the three-dimensional Anderson transition — •Alberto Rodriguez[1,2], Louella J. Vasquez[3], Keith Slevin[4], and Rudolf A. Roemer[2] — [1]Phisikalisches Institut, Albert-Ludwigs Universität Freiburg, 79104, Freiburg, Germany — [2]Department of Physics and Centre for Scientific Computing, University of Warwick, Coventry, CV4 7AL, UK — [3]Institute of Advanced Study, Complexity Science Centre and Department of Statistics, University of Warwick, Coventry, CV4 7AL, UK — [4]Department of Physics, Osaka University, 1-1 Machikaneyama, Toyonaka, Osaka 560-0043, Japan

We analyze the multifractal properties of the critical wavefunctions at the disorder-induced three-dimensional metal-insulator transition (MIT), and we discuss the relation between the multifractal spectrum and the probability density function (PDF) of wavefunction intensities at criticality. A new PDF-based characterization of the MIT is presented and emphasized in connection with latest experimental observations of critical phenomena. Furthermore, we describe a new multifractal finite size scaling (MFSS) procedure that permits the si-

multaneous estimation of the critical parameters and the multifractal exponents. Simulations of system sizes up to $L^3 = 120^3$ and involving nearly 10^6 independent wavefunctions have yielded unprecedented precision for the critical disorder $W_c = 16.530(16.524, 16.536)$ and the critical exponent $\nu = 1.590(1.579, 1.602)$. This formalism is applicable to any continuous phase transition exhibiting multifractal fluctuations in the vicinity of the critical point.