DY 25: Critical Phenomena and Phase Transitions

Time: Thursday 9:30–12:45 Location: H46

DY 25.1 Thu 9:30 H46

Computing melting temperatures of Na, Mg, Al and Si by pinning of solid-liquid interfaces in ab-initio calculations — •Felix Hummel[1], Ulf R. Pedersen[1,2], Georg Kresse[1], Gerhard Kahl[2], and Christoph Dellago[1] — [1]Faculty of Physics, University of Vienna, Boltzmanngasse 5, A-1090 Vienna, Austria — [2]Institute of Theoretical Physics, Vienna University of Technology, Wiedner Hauptstraße 8-10, A-1040 Vienna, Austria

We use a novel approach for computing the Gibbs free energy difference between phases of a material. The force acting on an interface separating two phases of interest is determined by applying an external field biasing two-phase configurations. This force is proportional to the Gibbs free energy difference between the phases.

We demonstrate the accuracy, efficiency and practical applicability of this approach by computing the melting temperature at ambient pressure of Na, Mg, Al and Si using ab-initio calculations with VASP. Whereas predicted melting temperatures are in good agreement with experiment for Na, Mg and Al, the melting temperature of Si is underestimated, in agreement with previous computations.

DY 25.2 Thu 9:45 H46

The role of phonons in the thermodynamics of Fe — •Michael Leitner[1,2], Jürgen Neuhaus[1,2], Karl Nicolaus[1], Winfried Petry[1,2], Bernard Hennion[3], and Arno Hiess[4] — [1]Technische Universität München, Physik Department E13, 85747 Garching, Germany — [2]Technische Universität München, Forschungs-Neutronenquelle Heinz Maier-Leibnitz (FRM II), 85747 Garching, Germany — [3]Laboratoire Léon Brillouin, CEA Saclay, 91191 Gif-sur-Yvette Cédex, France — [4]Institut Laue-Langevin, 38042 Grenoble, France, now at European Spallation Source AB, 22100 Lund, Sweden

We report measurements of the phonon dispersions for the three ambient-pressure phases of pure iron (α-Fe, γ-Fe and δ-Fe) by inelastic neutron scattering. Generally, the anharmonic effects lead to a softening of the phonons. Modelling the dispersions by a Born-von Kármán model with temperature-dependent force constants allows us to deduce the vibrational contributions to the energy and entropy differences at the phase transitions. We can conclude that while the latent heats arise mainly from the electronic contributions, the vibrational contributions to the entropy can not be neglected, and especially the $\gamma \leftrightarrow \delta$-transition is driven mainly by the increased vibrational entropy of the open bcc structure.

DY 25.3 Thu 10:00 H46

Critical Casimir forces between homogeneous and chemically striped surfaces — •Francesco Parisen Toldin[1], Matthias Tröndle[2], and Siegfried Dietrich[2] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg — [2]Max Planck Institute for Intelligent Systems, Heisenbergstr. 3, D-70569 Stuttgart

Recent experiments have measured the critical Casimir force acting on a colloid immersed in a binary liquid mixture near its continuous demixing phase transition, and exposed to a chemically structured substrate. Motivated by these experiments, we study the critical behavior of a system, which belongs to the Ising universality class, for the film geometry with one planar wall chemically striped, such that there is a laterally alternating adsorption preference for the species of the binary liquid mixture. By means of Mean-Field theory, Monte Carlo simulations and finite-size scaling analysis we determine the critical Casimir force and the corresponding universal scaling function.

DY 25.4 Thu 10:15 H46

Online discussions modeled by an evolving Ising-like dynamics — •Julian Sienkiewicz and Janusz Hołyst — Faculty of Physics, Center of Excellence of Complex Systems Research, Warsaw University of Technology, Poland

We present and exactly solve a one-dimensional model for emotional online discussions basing on the Ising-like asymmetrical and evolving dynamics. We restrict ourselves only to interactions with last message's emotions and study the dependence of the chain's average emotion $\langle e \rangle$ on external field h (community tendency toward a selected valence) and temperature T (uncertainty of the emotion). This leads us to an observation of three distinct phases - the first, where discussion evolution is determined by its beginning only, the second, in which the mostly observed emotion is coping the external influence, a finally, the third one, where the outcome is subject to fluctuations. The phases are separable with respect to the parameter that copies participant's uncertainty about their emotional behaviour.

DY 25.5 Thu 10:30 H46

MC test of cluster definitions in nucleation simulations of the lattice gas model — •Fabian Schmitz, Peter Virnau, and Kurt Binder — Johannes Gutenberg-Universität Mainz - Staudingerweg 7, D-55099 Mainz, Germany

The conventional theory of homogeneous and heterogeneous nucleation in a supersaturated vapor is tested by Monte Carlo simulations of the lattice gas (Ising) model with nearest-neighbor attractive interactions on the simple cubic lattice. The theory considers the nucleation process as a slow (quasi-static) cluster (droplet) growth over a free energy barrier ΔF^*, constructed in terms of a balance of surface and bulk term of a "critical droplet" of radius R^*, implying that the rates of droplet growth and shrinking essentially balance each other for droplet radius $R = R^*$.

Comparing different cluster definitions, namely geometrical clusters, Swendsen-Wang clusters and clusters applying the relations from classical nucleation theory, we find that, for all temperatures below the critical temperature, only the definition of "physical" clusters based on the Fortuin-Kasteleyn mapping is consistent with the estimates from the lever rule. The discrepancy between classical nucleation theory and the lever rule is determined for various temperatures.

DY 25.6 Thu 10:45 H46

Phase Transitions in Classical Lattice Gases with Three-Body Interactions — •Georg Maximilian Lohöfer — Institute for Theoretical Solid State Physics, RWTH Aachen University, Germany

We study a classical lattice gas on a honeycomb lattice in the parameter region where three-body interactions are dominant. Employing Monte Carlo simulations utilizing parallel tempering, we explore the complex low energy manifold, where highly-degenerate states for different values of the chemical potential emerge, resulting from the frustrated nature of three-body repulsions on the hexagonal lattice structure. We analyse the thermal phase transitions out of these low-temperature phases and identify a four-states Potts model transition that can be traced back to a partial re-ordering from an extensive ground state degeneracy at finite temperatures.

15 min. break

DY 25.7 Thu 11:15 H46

Continuous replica-symmetry breaking in mean-field spin-glass models: Perturbation expansion without the replica trick — Vaclav Janis, •Anna Kauch, and Antonin Klic — Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 18221 Praha, Czech Republic

The full mean-field solution of spin glass models with a continuous order-parameter function is not directly available and approximate schemes must be used to assess its properties. The averaged physical quantities are to be represented via the replica trick and the limit to zero number of replicas is to be performed for each of them. To avoid this we introduce a perturbation expansion for a mean-field free-energy functional with a continuous order-parameter function without the need to refer to the replica trick. The expansion can be used to calculate all physical quantities in all mean-field spin-glass models and at all temperatures, including zero temperature. The small expansion parameter is a difference between the continuous order-parameter function and the corresponding order parameter from the solution with one level of replica-symmetry breaking. The first correction beyond the approximation with one level of replica-symmetry breaking is explicitly evaluated in the glassy phase of the Sherrington-Kirkpatrick model.

DY 25.8 Thu 11:30 H46

Searching for spin-glass ground states in a transformed energy landscape — •Markus Manssen and Alexander K. Hartmann — Institut für Physik, Carl von Ossietzky Universität Oldenburg

Spin glasses and related models have been of interest to the scientific

community for decades due to their inherent disorder and frustration and the resulting complex energy landscape. But this at the same time makes time evolution of these systems particularly slow and finding the ground states very hard (for 3D systems NP-hard in fact [1]). Consequently many elaborate algorithms have been developed to tackle these problems. Karandashev et al. [2] have proposed an inverse approach in which one takes a power of a system's bond matrix, transforming its energy landscape to make finding the new ground state easier for any algorithm of choice. From there the original ground state should be easily reachable using the normal Hamiltonian. We test this method for the 3D binary Edwards-Anderson model with both the original authors preferred search algorithms and also Monte Carlo and parallel tempering simulations. We compare the results to the exact ground states. To evaluate the performance we have to also take the slow down caused by the transformed matrices into account.

[1] F. Barahona, On the computational complexity of Ising spin glass models, (J. Phys. A: Math. Gen. 15 3241, 1982)
[2] Ya.M. Karandashev and B.V. Kryzhanovsky, Transformation of energy landscape in the problem of binary minimization, (Doklady Mathematics, Vol. 80, No. 3, p. 927–931, 2009)

DY 25.9 Thu 11:45 H46

Stochastic Loewner evolution in the 2D Ising spin glass depends on boundary conditions — •Hamid Khoshbakht[1,2], 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 Centre, Coventry University, Coventry, CV1 5FB, UK — [3]University Chemical Laboratories, Lensfield Road, Cambridge, CB2 1EW, UK

Domain walls in two-dimensional Ising spin glasses are scale-invariant curves with fractal dimension d_f. Recent works indicate that $d_f \approx 1.27$ for Gaussian bond distribution and $1.09 \lesssim d_f \lesssim 1.39$ for bimodal couplings. In this contribution, we investigate whether the domain wall of this system satisfies Schramm-Loewner evolution (SLE) and is therefore also conformally invariant. Different boundary conditions are considered, and for each case d_f and the SLE diffusion constant κ of the corresponding Brownian motion are calculated. Correlations between different domain-wall segments are explicitly checked for by testing for independence of the increments of the Loewner driving function. The results show that changing the boundary conditions of the system does not change the fractal dimension, but the stronger conditions of SLE are only satisfied for specific choices of boundary conditions. In this sense, SLE is not universal.

DY 25.10 Thu 12:00 H46

Efficient Monte Carlo Simulations of the Random-Cluster Model using a Dynamic Connectivity Algorithm — •Eren M. Elçi and Martin Weigel — Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, England

The simulation of spin models close to points of continuous phase transitions is heavily impeded by the occurrence of critical slowing down. A number of cluster algorithms usually based on the Fortuin-Kasteleyn representation of the Potts model and suitable generalizations for continuous-spin models has been used to increase simulation efficiency. The first algorithm making use of this representation, suggested by Sweeny in 1983, has not found widespread adoption due to problems in its efficient implementation. It has been shown recently, however, that it is indeed more efficient in reducing critical slowing down that the more well-known variants due to Swendsen/Wang and Wolff. Here, we discuss an efficient implementation of Sweeny's approach using recent algorithmic advances in dynamic connectivity algorithms, and show how these can be used for efficient simulations in the random-cluster model. An extension of this approach, which is also efficient for first order phase transitions, is the combination of the random cluster model and multicanonical simulations. In this framework, we directly sample the combined geometrical bond- and cluster-number density of states of the model. By construction, this approach does not suffer from any (hyper-)critical slowing down.

DY 25.11 Thu 12:15 H46

Determination of line tension in the 3d Ising model using GPUs — •Benjamin Block, Suam Kim, Peter Virnau, and Kurt Binder — University of Mainz, Germany

Heterogeneous nucleation barriers are influenced by line tension effects [1]. We apply an efficient implementation of the Ising model on graphic cards [2] to quantify this effect in detail. In an Ising system with aperiodic boundary conditions in one dimension, a liquid vapor interface can be stabilized between two walls. When wall fields are applied, this leads to a difference in the Free Energy of the system. This change can be quantified in dependence on the linear dimensions of the simulation box and by varying the size of the box in all dimensions, the contribution of line tension can be extracted. [1] D. Winter, P. Virnau, K. Binder, PRL 103, 225703 (2009). [2] B. Block, EPJ-ST 210, 147 (2012).

DY 25.12 Thu 12:30 H46

Anisotropy and universality: Critical Binder cumulant of a two-dimensional Ising model — •Boris Kastening — Institute for Materials Science, Technische Universität Darmstadt, Germany

We reanalyze transfer matrix and Monte Carlo results for the critical Binder cumulant U^* of an anisotropic two-dimensional Ising model on a square lattice in a square geometry with periodic boundary conditions. Spins are coupled between nearest neighboring sites and between next-nearest neighboring sites along one of the lattice diagonals. We find that U^* depends only on the asymptotic critical long-distance features of the anisotropy, irrespective of its realization through ferromagnetic or antiferromagnetic next-nearest neighbor couplings [1]. Our results support our recent claim towards the validity of universality for finite-size scaling in the presence of a weak anisotropy [2].

[1] B. Kastening, arXiv:1209.0105.
[2] B. Kastening, Phys. Rev. E 86, 041105 (2012).