DY 18: Critical Phenomena and Phase Transitions

Time: Monday 15:30–17:00 Location: BH-N 333

DY 18.1 Mon 15:30 BH-N 333

Heterogeneous crystal nucleation on and far away from the pre-structured seeds — •Swetlana Jungblut — Physikalische Chemie, TU Dresden

We investigate the impact of the simultaneous presence of two seeds with various structures on the process of crystal nucleation in an undercooled Lennard-Jones fluid by means of computer simulations. In the presence of seeds with face- and body-centered cubic structures, we find that decreasing the inter-seed distance enhances the probability of the crystalline clusters formed on one of the seeds to grow beyond the critical size, thus, increasing the crystal nucleation rates. In contrast, when seeds have an icosahedral structure, the crystalline clusters form mostly in the bulk. The crystal nucleation rate, however, is also determined by the distance between the seeds, pointing to a heterogeneous crystal nucleation that occurs away from the icosahedrally structured seeds.

DY 18.2 Mon 15:45 BH-N 333

The plain and layered Ising spin glasses in two dimensions — •Martin Weigel[1], Hamid Khoshbakht[1,2], Mohammad-Sadegh Vaezi[3], Gerardo Ortiz[4], and Zohar Nussinov[3] — [1]Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, England — [2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, D-55099 Mainz, Germany — [3]Department of Physics, Washington University, St. Louis, MO 63160, USA — [4]Department of Physics, Indiana University, Bloomington, IN 47405, USA

The Ising spin glass in 2D exhibits rich behavior with subtle differences in the scaling for different coupling distributions. We use combinatorial optimization methods to determine exact ground states for systems with up to $10\,000 \times 10\,000$ spins. A combination of new algorithms allow us to treat samples with fully periodic boundaries and to sample uniformly from degenerate ground states for the $\pm J$ model. To establish a unified framework for studying both discrete and continuous coupling distributions, we introduce the *binomial* spin glass. In this model, the couplings are the sum of m identically distributed Bernoulli random variables. In the continuum limit $m \to \infty$, this system reduces to the Edwards-Anderson model with Gaussian couplings, while $m = 1$ corresponds to the $\pm J$ spin glass. Using this model, we derive a rigorous bound for the degeneracy of any energy level. Studying the defect energies in this model, we uncover intriguing subtleties in the behavior of the model with respect to the order in which the thermodynamic ($N \to \infty$) and continuum ($m \to \infty$) limits are taken.

DY 18.3 Mon 16:00 BH-N 333

Disassembling Casimir scaling functions at finite aspect ratios — •Hendrik Hobrecht and Fred Hucht — Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg

The finite-size scaling functions for the free energy of the two-dimensional Ising universality class are known exactly only either for finite aspect ratios at criticality due to conformal field theory (CFT), or for thin films at arbitrary temperatures. Beyond the thin films and CFT there are but a few results, namely for the torus, the open cylinder, and approaches for topologically more exotic forms like the open Möbius strip and the Klein bottle. Despite their role as potential for the critical Casimir force, even less is known in the presence of surface fields. We present a systematic calculation of the interlink between those limiting cases, implementing both symmetric (++) and asymmetric (+-) symmetry-breaking boundary conditions (BCs) on the cylinder with finite aspect ratio, as well as the often discussed Brascamp-Kunz BC. We show that the scaling limit of the latter one is indeed equal to open boundaries, as both are believed to represent Dirichlet BCs. An impressive feature of these scaling functions is the possibility to disassemble them not only into recurring bulk, surface, and finite-size contributions, but even beyond. We can distinguish different building blocks for the surfaces and surface fields, as well as for the breaking of the Z_2-symmetry and the surface tension due to imposed domain walls.

DY 18.4 Mon 16:15 BH-N 333

Analytic finite-size scaling functions in the anisotropic Ising rectangle — •Fred Hucht — Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg

The partition function of the square lattice Ising model on the rectangle, with open boundary conditions in both directions, is calculated exactly for arbitrary system size $L \times M$ and temperature. We start with the dimer method of Kasteleyn, McCoy & Wu, construct a highly symmetric block transfer matrix and derive a factorization of the involved determinant, effectively decomposing the free energy of the system into two parts, $F(L,M) = F_{\text{strip}}(L,M) + F^{\text{res}}_{\text{strip}}(L,M)$, where the residual part $F^{\text{res}}_{\text{strip}}(L,M)$ contains the nontrivial finite-L contributions for fixed M. While $F^{\text{res}}_{\text{strip}}(L,M)$ becomes exponentially small for large L/M or off-critical temperatures, it leads to important finite-size effects such as the critical Casimir force near criticality.

In the finite-size scaling limit $L, M \to \infty$, $T \to T_c$, with fixed temperature scaling variable $x \propto (T/T_c - 1)M$ and fixed aspect ratio $\rho \propto L/M$, we derive exponentially fast converging series for the related universal Casimir potential and Casimir force scaling functions. At the critical point $T = T_c$ we confirm predictions from conformal field theory. The presence of corners and the related corner free energy has dramatic impact on the Casimir scaling functions and leads to a logarithmic divergence of the Casimir potential scaling function at criticality.

A. Hucht, J. Phys. A: Math. Theor. **50**, 065201 (2017), arXiv:1609.01963; **50**, 265205 (2017), arXiv:1701.08722

DY 18.5 Mon 16:30 BH-N 333

Emergence of bistability in coupled spreading dynamics — •Fakhteh Ghanbarnejad — Institute of Theoretical Physics, Technical University of Berlin

In this work, we study different coupled spreading dynamics in an evolutionary ecological framework. Spreading of pathogens, fashions, ideas, products and so on are examples of such dynamical systems. These spreading phenomena are often coupled with each other in different ways: either to strengthen or weaken each other propagation. The coupling may lead to "nucleation" and as a consequence first order phase transitions at epidemic thresholds. Also it may lead to bi-stability in a wide regime of parameters [New J. Phys. 19, 103041(2017)]. Here we present examples of such scenarios from epidemiological modelling in mean filed approximations as well as simulations results on random generated networks. We also discuss which mechanisms may cause abrupt transitions in different time scales of the system [Frontiers in Physics, V 5, P 46 (2017)].

DY 18.6 Mon 16:45 BH-N 333

cooperative elastic self-amplification in molecular materials induced by ultrafast spin state photo-switching — •Roman Bertoni[1], Marco Cammarata[1], Hervé Cailleau[1], Maciej Lorenc[1], Eric Collet[1], and Cristian Enaschescu[2] — [1]University Rennes 1, UMR UR1-CNRS 6251, Rennes, France — [2]Faculty of Physics, Alexandru Ioan Cuza University, Iasi, Romania

The field of Photo-Induced Phase transition (PIPT) is reaching dynamical material control at fundamental time scale. Amongst molecular photo-switchable materials, spin crossover crystals are archetype of molecular bi-stability. We are now able to switch and control such systems at ultrafast time scale. The ultrafast photo-switching of these materials leads to a complex multistep out-of-equilibrium dynamics spanning from local molecular process to macroscopic material changes. The initial photo-switching process occurs within one picosecond at the local molecular scale involving coherent structural dynamics [1]. At longer time scale, the material response departs from that observed in diluted molecules due to the lattice action through structural feedback. Our new results have evidenced the existence of self-amplified elastic amplification during the volume expansion of the material inducing a multiplication of the fraction of molecules by factor five [3]. Such elastically-driven cooperativity triggered by a light pulse offers a new efficient way to generate and stabilize photo-induced phases in many volume-changing materials. [1]M. Cammarata et al, Phys. Rev. Lett 113, 227402 (2014)[2]R. Bertoni et al, Nature Materials 15 606-610 (2016)