DY 33: Critical Phenomena and Phase Transitions

Time: Wednesday 15:00–18:15 Location: BH-N 334

DY 33.1 Wed 15:00 BH-N 334

Fragmentation of fractal random structures — Eren M. Elçi, •Martin Weigel, and Nikolaos G. Fytas — Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, England

We analyze the fragmentation behavior of random clusters on the lattice under a process where bonds between neighboring sites are successively broken. Modeling such structures by configurations of a generalized Potts or random-cluster model allows us to discuss a wide range of systems with fractal properties including trees as well as dense clusters. We present exact results for the densities of fragmenting edges and the distribution of fragment sizes for critical clusters in two dimensions. Dynamical fragmentation with a size cutoff leads to broad distributions of fragment sizes. The resulting power laws are shown to encode characteristic fingerprints of the fragmented objects.

DY 33.2 Wed 15:15 BH-N 334

True asymptotics of self-avoiding walks on 3D percolation clusters. — •Niklas Fricke and Wolfhard Janke — Institut für Theoretische Physik and Centre for Theoretical Sciences (NTZ), Universität Leipzig, Postfach 100920, 04009 Leipzig, Germany

We study self-avoiding walks on three-dimensional critical percolation clusters using a new exact enumeration method. It overcomes the exponential increase in computation time by exploiting the clusters' fractal nature. We enumerate walks of over 10^4 steps, far more than has ever been possible. We found the scaling exponent ν for the end-to-end distance to be smaller than previously thought and the same on backbones and full clusters. Furthermore, we find strong evidence against the widely assumed scaling law for the average number of conformations and propose an alternative, which perfectly fits our data.

N. Fricke and W. Janke, arXiv:1410.5960, to appear in PRL (in print).

DY 33.3 Wed 15:30 BH-N 334

To return or not to return? Phase transition to transience and congestion in random walks and queueing systems — •Andreas Sorge[1,2,4], Jan Nagler[3,4], Stephan Herminghaus[1,2], and Marc Timme[1,2,4] — [1]MPI for Dynamics and Self-Organization, Göttingen, Germany — [2]Institute for Nonlinear Dynamics, Georg-August-Universität Göttingen, Germany — [3]Computational Physics, IfB, ETH Zürich, Switzerland — [4]Organization for Research on Complex Adaptive Systems (or-cas), Göttingen, Germany

Will a random walker ever return to where she started, and keep returning forever? When we are unaware of the law governing the walk, wisdom has it that we cannot infer recurrence from a finite-time sample trajectory. In 1890, Henri Poincaré introduced the very idea of such recurrences as a stability criterion. This criterion also applies to stochastic dynamical systems: By tuning the system parameter, a random walk loses recurrence and becomes unstable at a critical point. Intriguingly, this constitutes a phase transition to transience in Markovian systems. Here, we present a practical method to determine the critical point and the critical exponents of such systems in Monte-Carlo simulations. We also introduce the freely available Python implementation for effective and reproducible use of our method. Our findings and tools may be helpful in computational studies of stochastic systems, in particular queueing systems and dynamical congestion phenomena.

DY 33.4 Wed 15:45 BH-N 334

On the mixing of the single-bond dynamics for the random-cluster model — •Eren M. Elçi[1], Timothy Garoni[2], Andrea Collevecchio[2], and Martin Weigel[1] — [1]Applied Mathematics Research Centre, Coventry University, Coventry, CV1 5FB, England — [2]School of Mathematical Sciences, Monash University, Victoria, 3800, Australia

The Markov Chain Monte Carlo method is a ubiquitous tool in Statistical Physics. It is standard lore that close to a point of a second-order phase transition a phenomenon called critical slowing down hampers efficient sampling. A major breakthrough in reducing this slowing down for the random-cluster model has been the invention of the Swendsen-Wang-Chayes-Machta algorithm. Recently, however, it has been shown, that local chains can be as or even more efficient than non-local chains. Examples are the Worm algorithm for the Ising model and the single-bond dynamics for the random-cluster model. We present results of a numerical study of the coupling time of the single-bond chain dynamics for the random-cluster model. A careful analysis allows us to obtain high-precision (upper) bounds for auto-correlation, relaxation and mixing times for both critical and off-critical temperatures on square and simple-cubic lattices. The numerical results give strong evidence in favor of the rapid-mixing property of the single-bond dynamics for the random-cluster model, both at a second-order phase transition and off criticality. Furthermore we also present, to our knowledge, a novel heuristic method for detecting a first-order phase transition in the coupling-time distribution.

DY 33.5 Wed 16:00 BH-N 334

Nonstandard Finite-Size Scaling at First-Order Phase Transitions with Macroscopic Low-Temperature Phase Degeneracy — Marco Mueller[1], Desmond A. Johnston[2], and •Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany — [2]Department of Mathematics, School of Mathematical and Computer Sciences, Heriot-Watt University, Edinburgh EH14 4AS, Scotland, UK

We show that the standard inverse system volume scaling for finite-size corrections at a first-order phase transition (i.e., $1/L^3$ for an $L \times L \times L$ lattice in $3D$) is transmuted to $1/L^2$ scaling if there is an exponential low-temperature phase degeneracy. The gonihedric Ising model which has a four-spin interaction, plaquette Hamiltonian provides an exemplar of just such a system. We use multicanonical Monte Carlo simulations of this model to generate high-precision data which provides strong confirmation of the nonstandard finite-size scaling law. The dual to the gonihedric model, which is an anisotropically coupled Ashkin-Teller model, has a similar degeneracy and also displays the nonstandard scaling behaviour. A suitable "fuki-nuke" type order parameter and further potential applications of the transmuted finite-size scaling law will be briefly discussed.

M. Mueller, W. Janke, D.A. Johnston, Phys. Rev. Lett. **112** (2014) 200601;
M. Mueller, D.A. Johnston, W. Janke, Nucl. Phys. B **888** (2014) 214.

DY 33.6 Wed 16:15 BH-N 334

Phase transition of films in the Ising universality class — •Martin Hasenbusch — Humoldt-Universität zu Berlin, Deutschland

We study the phase transition of films with free and periodic boundary conditions. To this end we perform Monte-Carlo simulations of the Ising and the Blume-Capel model on the simple cubic lattice. Using a finite size scaling method, we determine accurately the transition temperature for thicknesses up to $L_0 = 64$. Since the transition is expected to share the universality class of the two-dimensional Ising model we can make use of exact and accurate numerical results obtained for this model. Our numerical results nicely confirm that the transition of the films indeed belongs to the universality class of the two-dimensional Ising model. We analyse how the transition temperature of the films approaches the transition temperature of the bulk system as the thickness increases. We confirm the power law behaviour predicted by finite size scaling.

15 min. break

DY 33.7 Wed 16:45 BH-N 334

Quantum phase transitions in networks of Lipkin–Meshkov–Glick models — •Aleksandr Sorokin, Victor Bastidas, and Tobias Brandes — Technische Universität Berlin, Berlin, Germany

The Lipkin–Meshkov–Glick (LMG) model describes an ensemble of all-to-all–coupled two-level systems with anisotropic interactions, exhibiting quantum phase transitions. In this contribution we show that coupling of several LMG systems with the overall Hamiltonian

$$\mathcal{H} = \sum_{l=1}^{N} \left[g J_l^z - \frac{\gamma}{2j} (J_l^x)^2 \right] - \frac{1}{2j} \sum_{l' \geq l=1}^{N} \kappa_{ll'} J_l^y J_{l'}^y$$

gives rise to phases with different collective behaviour. Namely, the weak-coupling regime corresponds to the paramagnetic phase when the local field dominates the dynamics, but the local anisotropy leads to the existence of an exponentially degenerate ground state. In the

strong-coupling regime, the ground state is twofold degenerate and possesses long-range magnetic ordering.

The calculations were performed in the mean-field (MF) approximation but taking into account quantum fluctuations around the MF solution. Within this approach analytical expressions for the ground-state and excitation energies as well as correlation functions in different phases were obtained for a network with the ring topology.

For details see [A V Sorokin, V M Bastidas and T Brandes, *Phys. Rev. E* **90**, 042141 (2014)]

DY 33.8 Wed 17:00 BH-N 334

Hypergeometric extrapolation of the strong coupling perturbation series of the Bose-Hubbard model — •Sören Sanders — Institut für Physik, Carl von Ossietzky Universität, D-26111 Oldenburg

Critical phenomena occuring at continuous phase transitions render a (low-order) perturbative description invalid. To overcome this a recently proposed scheme to obtain nonperturbative physics from low-order perturbation theory utilizing hypergeometric functions is studied and applied to the quantum phase transition from a Mott insulator to a superfluid undergone by the Bose-Hubbard model. The well-known phase diagram is reproduced and critical exponents obtained that are in remarkable agreement with the universality hypothesis.

DY 33.9 Wed 17:15 BH-N 334

Casimir force scaling functions in 2d Ising systems with open boundaries: The importance of corner contributions — •Fred Hucht and Felix M. Schmidt — Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg

We consider the two-dimensional square lattice Ising model with free boundary conditions, aiming at universal critical Casimir force scaling functions. Surprisingly, no closed form solution exists for finite $L_\parallel \times L_\perp$ lattices due to the lack of translational invariance in both directions. However, the exact partition function polynomial can be efficiently calculated from the determinant of a $(4L_\parallel L_\perp)$-dimensional sparse matrix using arbitrary-precision integer arithmetics. For infinite systems, we derive exact expressions for the bulk, surface and corner free energies at arbitrary temperatures using q-products [1]. Combining these results, we derive universal finite-size-scaling functions of the Casimir force and the residual free energy for different values of the aspect ratio $\rho = L_\perp/L_\parallel$. We find a unusual logarithmic divergence of the residual free energy scaling function at $x = tL_\perp \to 0$, which is directly related to the logarithmic L-dependence of the free energy at criticality predicted by Cardy and Peschel [2].

[1] E. Vernier and J. L. Jacobsen, J. Phys. A: Math. Theor. 45, 045003 (2012).

[2] J. Cardy and I. Peschel, Nucl. Phys. B 300, 377 (1988).

DY 33.10 Wed 17:30 BH-N 334

Thermodynamic properties of two-dimensional colloidal crystals with dipolar interactions — •Sven Deutschländer[1], Tobias Horn[2], Antonio Manuel Puertas[3], Hartmut Löwen[2], Georg Maret[1], and Peter Keim[1] — [1]University of Konstanz, Konstanz, Germany — [2]Heinrich-Heine-University Düsseldorf, Düsseldorf, Germany — [3]University of Almeria, Almeria, Spain

Colloidal suspensions provide the possibility to study a variety of classical many particle systems like glasses, gels, crystals or liquids on a microscopic scale by means of single particle resolution. Hence, macroscopically significant thermal and mechanical properties can be reasoned by the explicit structure and dynamics of the particles. By colloidal experiments and Monte Carlo simulations, we study the equilibrium melting scenario of two-dimensional systems with a repulsive dipole-dipole potential. Our results are largely in agreement with theoretical predictions of the continuous KTHNY melting scenario, but also indicate new prospects which are beyond the microscopic defect theory.

[1] S. Deutschländer, A. M. Puertas, G. Maret, and P. Keim, Phys. Rev. Lett. 113, 127801 (2014). [2] S. Deutschländer, T. Horn, H. Löwen, G. Maret, and P. Keim, Phys. Rev. Lett. 111, 098301 (2013). [3] T. Horn, S. Deutschländer, H. Löwen, G. Maret, and P. Keim, Phys. Rev. E 88, 062305 (2013)

DY 33.11 Wed 17:45 BH-N 334

Thermal and nonthermal phase transitions in silicon induced by femtosecond free-electron laser pulse — •Nikita Medvedev[1], Zheng Li[1,2], and Beata Ziaja[1,3] — [1]CFEL at DESY, Notkestr. 85, 22607 Hamburg, Germany — [2]University of Hamburg, 20355, Hamburg, Germany — [3]Institute of Nuclear Physics, Polish Academy of Sciences, Radzikowskiego 152, 31-342 Krakow, Poland

Silicon under irradiation with intense femtosecond laser pulses can undergo a phase transition via two different channels: thermal and nonthermal. The first one occurs if the lattice is heated strongly enough with electron-phonon coupling to trigger silicon melting, while the second one results from the modification of the interatomic potential energy surface by excitation of electrons from the valence to the conduction band. We developed a model to include both channels. Tight-binding molecular dynamics (TBMD) is used to model atomic dynamics with the potential dependent on the state of electronic system. Simultaneously, electronic state is traced with the Boltzmann equation for low-energy electrons (the valence and the bottom of the conduction band), and with a Monte Carlo model for photoabsorbtion, high-energy electrons, and deep shell holes.

Our results show that electron-phonon coupling triggers phase transition into a low-density liquid phase for the deposited doses > 0.65 eV/atom. For deposited doses of over 0.9 eV/atom, silicon undergoes a phase transition into high-density liquid phase triggered via interplay of thermal heating and the nonthermal change of the atomic potential.

DY 33.12 Wed 18:00 BH-N 334

Line contribution to the critical Casimir force between a homogeneous and a chemically stepped surface — •Francesco Parisen Toldin[1], Matthias Tröndle[2,3], and Siegfried Dietrich[2,3] — [1]Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Germany — [2]Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany — [3]IV. Institut für Theoretische Physik, Universität Stuttgart, Germany

Recent experimental realizations of the critical Casimir effect have been implemented by monitoring colloidal particles immersed in a binary liquid mixture near demixing and exposed to a chemically structured substrate consisting of stripes with alternating adsorption preferences, forming chemical steps between them. We analyze the contribution of such chemical steps to the critical Casimir force for the film geometry and within the Ising universality class. By means of Monte Carlo simulations, mean-field theory, and finite-size scaling analysis we determine the universal scaling function associated with the contribution to the critical Casimir force due to individual, isolated chemical steps facing a surface with homogeneous adsorption preference or with Dirichlet boundary condition. These results allow one to compute the critical Casimir force in the presence of arbitrarily shaped, but wide stripes as a sum of the contributions due to the homogeneous parts of the surface and due to the chemical steps between the stripes. We assess this decomposition by comparing the resulting sum with actual simulation data in the presence of a chemically striped substrate.
Ref: F. Parisen Toldin, M. Tröndle, S. Dietrich, arXiv:1409.5536