DY 13: Statistical Physics (general)

Time: Monday 15:00–17:15 Location: H48

DY 13.1 Mon 15:00 H48

Numerische Simulation zur Hochtemperatur-Supraleitung — •Ingo Morgenstern — Universtätsstraße 31, 93053 Regensburg

Gezeigt werden numerische Simulationen zum Hubbard-Modell in zwei Dimensionen für U=2 und U=3. Verwendet wird ein auf dem Weltrekordalgorithmus (2009 weltweit eine der besten 50 Erfindungen) basierendes Verfahren mit korrekter Mitnahme des Minussigns. Das Modell zeigt in diesem Falle Hochtemperatur-Supraleitung. Für größere U bricht die Simulation zusammen. Ein Bias im Minussign unterdrückt darüber hinaus die Supraleitung. Es wird gezeigt, dass die nichtlineare Ankopplung des Apex-Sauerstoffs zu einer Absenkung der effektiven Hubbard-Abstoßung zu Werten von U=3 vom realistischen Wert führt. Damit ist der Apex-Sauerstoff nicht ursächlich für die Hochtemperatur-Supraleitung verantwortlich, sondern nur für die Absenkung des effektiven Us. Andere Mechanismen, die ebenfalls in ein effektives U zwischen 2 und 3 verursachen, führen demnach auch zu Hochtemperatur-Supraleitung.

DY 13.2 Mon 15:15 H48

Determining the size at which neutral gold clusters turn three-dimensional at finite temperature — •Bryan Goldsmith[1], André Fielicke[2], Matthias Scheffler[1], and Luca Ghiringhelli[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany — [2]Institut für Optik und Atomare Physik, Technische Universität Berlin, Hardenbergstrasse 36, D-10623 Berlin

Discerning the ground state structure of free gold clusters, and in particular the critical size when Au clusters begin favoring three-dimensional (3D) structures over planar structures at 0 K, has been a topic of longstanding interest. At finite temperature, however, Au clusters exhibit coexistence of many structural isomers. To move beyond the monostructure description of clusters at 0 K, we performed *ab initio* replica-exchange molecular dynamics (REMD) on Au_n clusters (n=5-14) to identify metastable states, their relative stability, and to examine the influence of entropy and van der Waals (vdW) on the isomer energetics. REMD calculations used PBE with the scalar ZORA correction and either Tkatchenko-Scheffler or Many-Body-Dispersion vdW. Free energies of Au isomers are estimated using the Multistate Bennett Acceptance Ratio and the planar and 3D isomer populations are examined between 100-1000 K. The distribution of bond coordination numbers is used to discriminate isomers along the dynamical trajectories. Isomer energetic ordering is verified using renormalized second-order perturbation theory. Computed anharmonic IR spectra of Au_n are compared with experimental spectra.

DY 13.3 Mon 15:30 H48

Effects of Local Measurements on Quantum Statistical Ensembles — •Walter Hahn[1] and Boris Fine[1,2] — [1]Institute for Theoretical Physics, University Heidelberg, Germany — [2]Skolkovo Institute of Science and Technology, Moscow, Russia

We investigate the effect of local measurements on quantum statistical ensembles for macroscopic systems. The system chosen is a lattice of spins 1/2 subject to projective measurements of individual spins. We find that the effect of measurements depends on system's Hamiltonian and on the initial statistical ensemble. The above findings justify prescriptions for protecting unconventional statistical ensembles.

DY 13.4 Mon 15:45 H48

Q–tensor Density Functional Theory of Non–spherical Hard–Body Mixtures — •Rodrigo Lugo-Frias and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany

In nature there are numerous examples of polydisperse systems composed of molecules with different shapes and concentrations. The behavior of these complex fluids in and out of equilibrium is a long–standing problem with relevance in material science, engineering and soft matter theory.

On the basis of density functional theory and the phase–field–crystal model for liquid crystals [1] we derive in detail a free energy functional of an N component hard–body mixture in terms of a set of tensorial order parameters $\{\mathbf{Q}^i\}$. In contrast to previous works on binary non–spherical mixtures [2], our free energy functional includes gradients of the order parameters. Thus, our description can be used as a starting point to explore liquid–crystalline phases of mixed systems with spatial inhomogeneities, or as an input to mesoscopic dynamical equations for the orientational order parameters.

[1] R. Wittkowski, H. Löwen and H. R. Brand, Phys. Rev. E, **82**, 031708 (2010).
[2] R. Lugo-Frias and S. H. L. Klapp, J. Phys.: Condens. Matter, *submitted* (2015).

DY 13.5 Mon 16:00 H48

From Shapiro-Steps to frozen Kinks — •Thorsten Brazda and Clemens Bechinger — Pfaffenwaldring 57, 70550 Stuttgart, Germany

Although friction is ubiquitous in our everyday lives, a microscopic understanding is still lacking. This is partially due to the small length scales, which are not easily accessible in experiments. To overcome this problem and to observe individual particle motion during sliding, we studied a two-dimensional commensurate colloidal crystal which is driven across a (111) substrate, the latter created by a laser interference pattern [1]. In order to study the effect of substrate lattice vibrations on the sliding motion we have periodically modulated the substrate strength U. For small driving forces F, we observe a cooperative, phase-locked, particle motion which leads to characteristic Shapiro-steps in the mobility-force plane. At higher F, the colloids form an increasing number of local compression zones (kinks) which are still mobile during time-intervals where U is small. On the contrary, for large U, the particle motion is entirely stopped and the kinks are frozen. The formation of kinks leads to an incoherent particle motion which leads to the blurring of Shapiro-steps until they finally disappear at high F.

[1] T. Bohlein J. Mikhael and C. Bechinger, Observation of kinks and antikinks in colloidal monolayers driven across ordered surfaces, Nat. Mater. 11, 126 (2011).

DY 13.6 Mon 16:15 H48

Melting in 2D and a Fresh Perspective on Monte Carlo — •Sebastian Kapfer[1] and Werner Krauth[2] — [1]Theoretische Physik 1, FAU Erlangen — [2]LPS, Ecole Normale Superieure, Paris

The melting transition of two-dimensional solids has been the subject of continued research for more than fifty years, with the prevalent scenarios being the KTHNY theory of defect unbinding and a conventional first-order liquid/solid transition. For hard disks, the KTHNY scenario has recently been essentially confirmed, even though the liquid-hexatic step is of first order [1]. A key problem in these simulations are the large correlation lengths, which we tackle using a new rejection-free global-balance Monte Carlo algorithm [2].

We show that the hard disk result transfers to soft interactions with inverse power-law or Yukawa potentials [3]. The order of the liquid-hexatic step can be tuned from first-order to continuous by softening the potential. We show that there is always a hexatic phase separating the liquid and solid phases, and identify two regimes of the hexatic with vastly different correlation lengths.

The new algorithm is very versatile, and could also be applied to spin systems, polymers, path integral problems, etc. It can be augmented to treat long-range force laws such as Coulomb without any artificial truncation.

[1] E. P. Bernard, W. Krauth, Phys. Rev. Lett. 107, 155704 (2011). [2] M. Michel et al., J. Chem. Phys. 140, 054116 (2014). [3] S. C. Kapfer, W. Krauth, Phys. Rev. Lett. 114, 035702 (2015).

DY 13.7 Mon 16:30 H48

Apparent non-universality due to competing anisotropies in 3D Zq models — •Thomas Lottermoser[1], Andres Cano[2], and Manfred Fiebig[1] — [1]Department of Materials, ETH Zürich, Vladimir-Prelog-Weg 4, 8093 Zurich, Switzerland — [2]CNRS, Université de Bordeaux, ICMCB, UPR 9048, 33600 Pessac, France

3D Z_q models ($q > 4$) like the q-state clock model, antiferromagnetic Potts model or the XY model with discrete q-fold anisotropy, are known to belong all to the XY-universality class at criticality, whereas the Z_q anisotropy is dangerously irrelevant at T_C. This leads to a new length scale associated to the fluctuations of the phase of the order

parameter with a critical exponent $\nu_q > \nu$. Here ν is the standard XY critical exponent for the correlation length ξ of the order parameter amplitude. While there is a general agreement on this behavior in the literature, due to contradicting simulation results the question of the universality of ν_q aroused. We propose that these contradictions can be explained by the existence of competing anisotropies. Therefore, in our extensive Monte-Carlo study we investigated the critical behavior of a 12-state clock model with competing 6-fold anisotropy. As a result we found that the apparent non-universality of ν_q can indeed be traced back to the strength of the competing anisotropy we introduced in our model system. This allows us to continuously tune the value of ν_q between the universal values for the 6-state and 12-state clock models, respectively.

DY 13.8 Mon 16:45 H48

Analytical one-dimensional approach of understanding water anomalies and phase transitions — •Katharina Ferling and Andreas Heuer — Institut für Physikalische Chemie, WWU Münster, Germany

The understanding of the water behaviour, including its anomalies, can play an important role in improving the description of water. Here the emphasis lies on the property of building H-bonds which is believed to be one major factor for many anomalies such as the density change or the liquid-liquid phase transition at low temperatures. For the present investigation a simple model has been chosen which focuses on the distinction between a close-packed and an open structure. The one dimensional model - which was first introduced by Ben-Naim [1] - has now been extended by terms, capturing the interaction of second-nearest neighbours as well as the transition to the gas phase at high temperatures. Here, two different analytical approaches are evaluated via explicit calculation of the partition function, and selected properties are discussed with the aim to show water-like behaviour such as a high-density liquid and low-density liquid (HDL-LDL) transition. One model shows a clear first order phase transition between a high-density and a low-density phase and both models have a (theoretical) transition line with negative slope in the p-T plane. Furthermore, anomalous behaviour of several properties, such as the density, heat capacity and isothermal compressibility, is visible, as can be seen in real water.

[1] Arieh Ben-Naim, J. Chem. Phys. 128, 024505 (2008)

DY 13.9 Mon 17:00 H48

Metadynamics for Nucleation studies in Potts-Models — •Ralf Schmid and Peter Nielaba — Universität Konstanz, Konstanz, Baden-Württemberg

Simulating nucleation processes in particle based systems can be time consuming due to large barriers in the free energy landscape. So new simulation techniques like Umbrella Sampling, Thermodynamic Integration and Metadynamics were invented for accelerating rare events. In molecular dynamics studies of nucleation the Metadynamics protocol was successfully used to accelerate the process and to calculate the free energy landscape in given reaction coordinates like cluster size.

We use the Metadynamics tool in Potts-Model systems to study nucleation and crystallization. The underlying dynamics of the system is a Metropolis Monte-Carlo simulation in the semi-grand canonical ensemble. The use of different reaction coordinates leads to insights into the basic processes that enable nucleation.