DY 2: Statistical Physics (general)

Time: Monday 10:15–13:15 Location: ZEU 255

DY 2.1 Mon 10:15 ZEU 255

A new factorizacion form for the partition function in quantum open systems — •Juan-Diego Urbina and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, D-93053 Regensburg, Germany

We adress the microscopic description of quantum systems strongly coupled with a linear bath (particularly at very low temperatures) in the framework of the Caldeira-Legget model for the environment. By careful revision of the huge literature on the subject, we support our claim that a weak coupling assumption is inconsistenly done at a very critical stage in basically all thermodynamic calculations. This extra assumption (based on its exactness for harmonic systems) is expressed through a factorized form for the full system-plus-environment equilibrium partition funtion $Z(\beta)$, in terms of the partition function of the bath $Z_{B}(\beta)$ and the effective partition function of the system $Z_{eff}(\beta)$. We will show how the explicit construction of the full partition function of a non-harmonic system (the particle in a box interacting with a bath of harmonic oscilators) suggests a different picture where an extra universal factor, representing neither the system nor the bath but the interaction between them, is naturally added to $Z(\beta)$.

DY 2.2 Mon 10:30 ZEU 255

Canonical thermalization — •Peter Reimann — Universität Bielefeld

For quantum systems which are weakly coupled to a much bigger environment, thermalization of possibly far from equilibrium initial ensembles is demonstrated: for sufficiently large times, the ensemble is for all practical purposes indistinguishable from a canonical density operator under conditions that are satisfied under many, if not all, experimentally realistic conditions [1].

[1] P. Reimann, New J. Phys. 12, 055027 (2010); Phys. Rev. Lett. 101, 190403 (2008)

DY 2.3 Mon 10:45 ZEU 255

Generalization of the parQ method to the grand canonical ensemble — •René Haber and Karl Heinz Hoffmann — Institut für Physik, Technische Universität Chemnitz, 09107 Chemnitz, Germany

We present the extension of our transition matrix Monte Carlo method parQ[1] to the grand canonical ensemble. It calculates the density of states $g(E, N)$ in a given energy and particle-number range from transition data. The method is easily parallelizeable, as one can fill the transition matrix from independent simulations running on different processors. It is also flexible in terms of the sampling scheme used as it can be adopted to standard Metropolis sampling, parallel tempering, Wang-Landau sampling as well as probably other sampling methods. At the end of the simulation the eigenvector corresponding to the eigenvalue 1 is calculated, which can be identified as the density of states. Results from simulations of simple Lennard-Jones systems as well as more complex hexadecane systems are presented.

[1] F. Heilmann and K. H. Hoffmann. Europhysics Letters, 70(2):155-161, 2005.

DY 2.4 Mon 11:00 ZEU 255

Binary nucleation: molecular dynamics simulation of the n-nonane/methane system — •Stephan Braun and Thomas Kraska — Institute of Physical Chemistry, University of Cologne, Luxemburger Str. 116, D-50939 Köln

Molecular dynamics simulation is employed to investigate the vapour-liquid nucleation of the binary system n-nonane/methane. The supersaturation of the system is achieved by cooling down the system during expansion in order to closely mimic the real process which is in practice applied, for example, to separate heavy compounds from natural gas.

By means of molecular dynamics simulations it is possible to obtain several details of the nucleation process, which are difficult or impossible to obtain from experiments. This regards the early stages of nucleation and growth taking place on the nanosecond time scale. Properties such as the nucleation rates or the critical cluster size can be determined even at high pressures. Furthermore, the determination of the composition of the clusters and the cluster structure can help to understand the nucleation process. Simulations where performed at different temperatures and densities for systems with various molefractions. The resulting nucleation rates have been compared to nucleation theory and the obtained clusters where analyzed with regard to structure and composition to understand possible effects on the nucleation process.

DY 2.5 Mon 11:15 ZEU 255

Non-metal-to-metal transition driven by van der Waals forces in an interacting polaronic gas — •Pascal Quémerais[1,2] and Gennady N. Chuev[3,4] — [1]Institut Néel, CNRS-UJF, Grenoble, France — [2]Max-Planck-Institute for Physics of Complex Systems, Dresden, Germany — [3]Russian Academy of Science, Pushchino, Moscow Region, Russia — [4]Max-Planck-Institute for Mathematics in the Sciences, Leipzig, Germany

We develop a model treating non-degenerate Fröhlich polarons with long-range Coulomb interactions at low densities and temperatures. Starting from the dilute regime, we show that at strong electron-phonon coupling, the collective properties of polarons are mainly governed by dipolar interactions in the crystallized state (Polaron Wigner Crystal) at zero temperature. At larger temperature in the liquid state, the dipolar interactions corresponds to the London dispersion forces, i.e. induced dipole-dipole van der Waals interactions. At a critical density, these forces provoke a non-metal to-metal transition by means of a polarization catastrophe which results in a polaron dissociation. The 3D and 2D case will be discussed as well as possible applications to real systems (metal-ammonia solutions, high-Tc cuprates).

[1] G.N. Chuev, P. Quémerais *J. Chem. Phys.* **127**,244501 (2007)
[2] G.N. Chuev, P. Quémerais *J. Chem. Phys.* **128**, 144503 (2008)
[3] P. Quémerais, G.N. Chuev, *New Jour. Phys.* **12** 023030 (2010)

DY 2.6 Mon 11:30 ZEU 255

Domain walls and Schramm-Loewner evolution in the random-field Ising model — •Jacob Stevenson and Martin Weigel — Johannes Gutenberg Universität, Mainz

The concept of Schramm-Loewner evolution provides a unified description of domain boundaries of many lattice spin systems in two dimensions, possibly even including systems with quenched disorder. Here, we study domain walls in the random-field Ising model. Although, in two dimensions, this system does not show an ordering transition to a ferromagnetic state, in the presence of a uniform external field spin domains percolate beyond a critical field strength. Using exact ground state calculations of very large systems, we examine ground state domain walls near this percolation transition finding strong evidence that they are conformally invariant and satisfy the domain Markov property, implying compatibility with Schramm-Loewner evolution with parameter $\kappa = 6$. These results might pave the way for new field-theoretic treatments of systems with quenched disorder.

15 min. break.

DY 2.7 Mon 12:00 ZEU 255

Monte Carlo simulations without detailed balance — •Martin Weigel[1] and Heitor Fernandes[2] — [1]Institut für Physik, KOMET 331, Johannes Gutenberg-Universität Mainz, Staudinger Weg 7, 55127 Mainz — [2]Instituto de Física, Universidade Federal do Rio Grande do Sul, CP 15051, 91501-970 Porto Alegre RS, Brazil

Monte Carlo simulations are used to study simple systems where the underlying Markov chain satisfies the necessary condition of global balance but does not obey the more restrictive condition of detailed balance. Here, we show that non-reversible Markov chains can be set up that generate correct stationary distributions, but reduce or eliminate the diffusive motion in phase space typical of the usual Monte Carlo dynamics. Our approach is based on splitting the dynamics into a set of replicas with each replica representing a biased movement in reaction-coordinate space. This introduction of an additional bias in a given replica is compensated for by choosing an appropriate dynamics on the other replicas such as to ensure the validity of global balance. First, we apply this method to a mean field Ising model, splitting the system into two replicas: one trying to increase magnetization and

the other trying to decrease it. For this simple test system, our results show that the altered dynamics is able to reduce the dynamical critical exponent. Generalizations of this scheme to simulations of the Ising model in two dimensions are discussed.

DY 2.8 Mon 12:15 ZEU 255

Magnetic Friction: Stokes to Coulomb — •Sebastian Angst, Martin P. Magiera, Alfred Hucht, and Dietrich E. Wolf — Fakultät für Physik, Universität Duisburg-Essen, D-47057 Duisburg

In recent years, the interest in magnetic contribution to friction due to spin correlations has been increased. One intriguing aspect is the energy dissipation by reason of spin waves induced by a moving tip above a substrate of Heisenberg spins [1], modeled with the Landau-Lifshitz-Gilbert equation. In addition, magnetic friction occurs in a driven Ising model [2] investigated by using Monte-Carlo simulations and analytical methods [3]. Until now the dependency of the friction force f on the velocity v is characterized by a Stokes-like behavior for Heisenberg spins and a Coulomb-like behavior for the Ising model.

Here we show that the qualitative characteristics of $f(v)$ are independent on model details like the spin dimensionality, the model geometry or the simulation methods. Using an Ising model in a moving field of different shapes, we demonstrate that the relevant quantity is the time evolution of the field at a given site [4].

[1] M.P. Magiera et al., EPL 87, 26002 (2009)
[2] D. Kadau et al., Phys. Rev. Lett. 101, 137205 (2008)
[3] A. Hucht, Phys. Rev. E 80, 061138 (2009)
[4] to be published

DY 2.9 Mon 12:30 ZEU 255

Atomistic Modeling of Electromigration — •Andreas Latz and Dietrich E. Wolf — Fakultät für Physik, Universität Duisburg-Essen, D-47057 Duisburg

Strong electric fields lead to a directed movement of atoms in a current carrying conductor. This mass transport is called electromigration and is induced by interactions of the conducting electrons (wind force) and the electric field (direct force) with the atoms. Due to the high current densities ($10^6 \mathrm{A/cm}^2$) in integrated circuits, electromigration-induced short circuits and voids are a problem.

We use the Kinetic Monte Carlo method to simulate the dynamics of voids in silver nanowires at the atomic scale. The dependence of the void form on the crystallographic orientation of the nanowire and the direction of the electric field will be shown. In a (001)-oriented silver wire squarelike voids can be observed, in contrast to a (111)-oriented wire, in which voids are triangular and pointed in migration direction. The simulation results are in agreement with experimental observations made with monocrystalline silver nanowires in the SFB 616 "Energy dissipation at surfaces".

Topical Talk DY 2.10 Mon 12:45 ZEU 255

Trends, questions and methods in molecular magnetism — •Jürgen Schnack — Universität Bielefeld, Universitätsstr. 25, D-33615 Bielefeld

The field of molecular magnetism has seen a rapid development during the past 15 years. Initially driven by the discovery of slow magnetic relaxation and magnetic hysteresis on the molecular level, the field nowadays spreads out into several directions as for instance quantum manipulation of molecular qubits, manipulation and investigation of deposited magnetic molecules, rational design of magnetic molecules with large anisotropy barriers or with large ground-state degeneracies for huge magnetocaloric effects. Such activities rise questions of reachable decoherence times or addressability of deposited molecules as well as of methods to theoretically describe both the molecules as well as the desired processes. Theoretical descriptions, that mostly aim at a complete quantum description, have advanced a lot in the field. A few of them will be highlighted.