DY 2: Statistical Physics (General)

Time: Monday 9:30–12:45 Location: MA 004

Invited Talk DY 2.1 Mon 9:30 MA 004

Separation of chiral particles in micro- and nanofluidic systems — •Ralf Eichhorn — Nordic Institute for Theoretical Physics (Nordita), Stockholm, Sweden

Standard techniques for separating a mixture of chiral molecules (enantiomers) rely on chiral auxiliary substances. We discuss the alternative possibility to sort chiral molecules by their distinct physical behavior in external force fields without making use of additional chiral agents. Using numerical simulations and theoretical arguments, this separation concept is demonstrated for simple model systems, and the basic physical mechanisms are illustrated and analyzed. Furthermore, experimental realizations in microfluidic systems are presented.

DY 2.2 Mon 10:00 MA 004

Kinetics of Nucleation on Surfaces in the Ising model — •Fabian Schmitz, Peter Virnau, and Kurt Binder — Institut für Physik, Johannes Gutenberg-Universität Mainz - Staudingerweg 7, D-55099 Mainz, Germany

We consider homogeneous and heterogeneous nucleation in the 3d Ising model, and compare information gained from nucleation dynamics to free energy computations in the context of classical nucleation theory. To define "physical clusters", the Swendsen-Wang algorithm is applied. We force the system into a metastable state from which it escapes into a stable state via nucleation. In the heterogeneous case, two flat walls with surface fields are introduced on which nuclei grow with some contact angle depending on the surface fields. To extract the critical cluster size, at which clusters decay or grow with equal probability, we measure the average growth rate $R(l)$ of nuclei with size l by monitoring the growth and decay of individual clusters over time for varying bulk and surface magnetic fields. Critical cluster sizes obtained from this method are comparable yet slightly larger than predicted from classical nucleation theory in both homogeneous and heterogeneous nucleation scenarios. The time dependence of the cluster distributions are also in agreement with previous predictions.

DY 2.3 Mon 10:15 MA 004

Explosive condensation in a mass transport model — •Bartlomiej Waclaw and Martin Evans — School of Physics, University of Edinburgh

Recent studies in non-equilibrium statistical physics show that diverse phenomena such as jamming in traffic flow, wealth condensation in macroeconomies or hub formation in complex networks can be understood by the condensation transition, in which a finite fraction of the system mass becomes localized in space. A classical model of condensation is the Zero-Range Process (ZRP) in which particles hop between sites of a 1d lattice with the rate which decreases with the number of particles at the departure site. This causes the condensate to evolve more slowly, the more particles it has. Therefore, the condensate remains static once it has formed, melting and reforming very rarely. In his talk we demonstrate a completely different mechanism of condensation, motivated by processes such as gravitational clustering or formation of droplets in clouds, where aggregation of particles speeds up in time as a result of increasing exchange rate of particles between growing clusters. In our model, particles hop between lattice sites with the rate u(m,n) which increases with the numbers m,n of particles at interacting sites. We show that condensation occurs in this model through a contrasting dynamical mechanism to that previously considered — the formation of the condensate happens on a very fast time scale and we term it explosive.

DY 2.4 Mon 10:30 MA 004

Flexible Rare Event Sampling Harness System — •Kai Kratzer and Axel Arnold — Institute for Computational Physics, Stuttgart, Germany

Many processes in nature can be classified as rare events, e.g. chemical reactions, nucleation of crystals or translocation of DNA through a pore. In all this processes, the time between the occurance of these events is much larger than the temporal duration of the event itself, meaning that practically all the simulation time is spent in waiting for the event. If the system under consideration requires expensive calculations, for example electrostatic interactions, the event will never happen using conventional brute-force simulations.

Recently, several new methods to succeed in this challenge have been put forward, particularly Forward Flux Sampling (FFS) or S-PRES. In this work, we present a flexible framework for simulating rare events using these sampling techniques. Our framework is suitable for simulating quasi-static and dynamic systems in the equilibrium or the non-equilibrium state and uses a plugin-system for the underlying dynamics. At present, it can steer popular MD packages such as GROMACS, ESPResSo, but due to the simple interface of our plugin-system, it is also easy to attach other or self-written code. The system supports farming via standard TCP/IP networking and uses a database for efficient information storage. It is therefore also suited to make use of current parallel high performance hardware.

DY 2.5 Mon 10:45 MA 004

A new method to calculate partition functions — •Klaus Morawetz — Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics (IIP) Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

An exact correspondence is established between a N-body classical interacting system and a $N-1$-body quantum system with respect to the partition function. The resulting hermitian quantum-potential is a $N-1$-body one. Inversely the Kelbg potential is reproduced which describes quantum systems at a quasi-classical level. The found correspondence between classical and quantum systems allows also to approximate dense classical many–body systems by lower order quantum perturbation theory replacing Planck's constant properly by temperature and density dependent expressions. As an example the dynamical behavior of an one - component plasma is well reproduced concerning the formation of correlation energy after a disturbance utilizing solely the analytical quantum - Born result for dense degenerated Fermi systems. As further examples the application to spin models is discussed. K. Morawetz; Phys. Rev. E 66 (2001) 022103

15 min. break

DY 2.6 Mon 11:15 MA 004

An extension of the derivative expansion of the exact renormalization group to finite momenta — •Nils Hasselmann — MPI f. Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart

The non-perturbative renormalization group (NPRG) technique is based on an exact fow equation of the effective average action. It has proved especially useful when applied to critical phenomena. While the exact flow equation of the effective average action can almost never be solved, it allows for novel approximation techniques which are indeed non-perturbative. One rather successful approximation strategy is the derivative expansion, where the effective average action is expanded consistently to a given order in spatial derivatives, but no truncation is made in the power of the fields.

Here we present a simple truncation scheme of the exact flow equations for the effective action which allows to access the full momentum structure of vertices while at the same time reproducing the results of a leading order derivative expansion of the action, where local correlations are kept to infinite order in the fields. Different to existing schemes to calculate momentum dependent vertices, in our scheme all approximations are done at the level of the effective action which is generally better than truncating the flow equations of a field expansion. As an example for the feasibility of the technique, we present results for the O(n) model.

DY 2.7 Mon 11:30 MA 004

The Central Limit Theorem in Hierarchical Structures — •René Pfitzner, Pavlin Mavrodiev, Ingo Scholtes, Claudio J. Tessone, and Frank Schweitzer — Chair of Systems Design, ETH Zurich, Switzerland

In statistics the (classical) Central Limit Theorem for independent and identically distributed variables is well known. A generalization of this theorem is the so-called *Lyapunov Central Limit Theorem*, which is applicable to settings with independent, but *not* necessarily identically distributed random variables. In this contribution, we generalize these theorems in a hierarchical setting i.e., the aggregation of random variables is performed in a step-wise fashion where first sub-groups of all variables get aggregated. We show that the non-linearity introduced by the hierarchical organization of the variables leads to an interesting effect: not all the aggregation schemes lead to the same variance at the end of the hierarchy. In fact, there is an optimum hierarchical structure that minimizes the final error, or variance. We pose an optimization problem to find the "most-beneficial" hierarchical scheme for aggregation. We argue that our results have broad implications, ranging from the arrangement of measurements taken with devices with different intrinsic precision, to group decision making.

DY 2.8 Mon 11:45 MA 004

Stochastically driven Preisach models of hysteresis — •Sven Schubert and Günter Radons — Chemnitz University of Technology, 09107 Chemnitz, Germany

The Preisach model is a phenomenological model which is successfully applied to describe hysteretic interrelations of various physical and non-physical origins. Hysteresis involves the development of a memory which is accountable for the multistability present in such systems. It was shown recently [1] that this memory is reflected in long-time tails in the autocorrelation of the response of the Preisach model even for uncorrelated external driving fields. Hence, hysteresis is a mechanism for the generation of 1/f-noise. Using numerical simulations, these rigorous results are extended to models driven by Markovian input processes with finite correlation decay rate and by stochastic processes showing long-term correlations.

One observes that the autocorrelation of the hysteresis response does never decay faster than the autocorrelation of the external driving. We show that the rigorous results on Preisach models with uncorrelated input also hold asymptotically in presence of exponentially decaying input correlations. Furthermore, we show that uncorrelated driving fields can cause a slower correlation decay of the hysteresis response than long-term correlated driving fields.

[1] G. Radons, Phys. Rev. Lett. **100**, 240602 (2008).

DY 2.9 Mon 12:00 MA 004

Study of transistor performance of carbon nanotube networks — Milan Žeželj, •Igor Stanković, and Aleksandar Belić — Institute of Physics Belgrade, Scientific Computing Laboratory

In the random networks of mixed metallic and semiconducting carbon nanotube (CNT) with different chiralities, there is a trade off between high on-current (dense networks) and high on/off current ratio (sparse networks). Monte Carlo simulations were performed to study effects of nanotube/nanotube contact resistance on the on- and off-currents. Using tunneling model we confirm that junction conductance between two CNTs is strongly dependent on the crossing angle. The nanotubes exhibit a peak of conductivity over the different angular ranges depending on their chiralities. We analyze how percolation threshold density of CNTs, conductivity exponents and prefactors depend on the position and width of conductive peak. Furthermore, when network size is comparable to a single CNT length, we find a significant size dependence of the on/off currents and their variance.

Invited Talk DY 2.10 Mon 12:15 MA 004

Melting transition of hard disks — •Werner Krauth — Departement de physique, Ecole normale superieure, Paris, France

The hard-disk model has exerted outstanding influence on computational physics and statistical mechanics. Decades ago, hard disks were the first system to be studied by Markov-chain Monte Carlo methods and by molecular dynamics. It was in hard disks, through numerical simulations, that a two-dimensional melting transition was first seen to occur even though such systems cannot develop long-range crystalline order. Analysis of the system was made difficult by the absence of powerful simulation methods.

In recent years, we have developed a number of powerful Monte Carlo algorithms for hard disks and related systems. I will in particular show how the powerful event-chain Monte Carlo algorithm has allowed us to prove that hard disks melt with a first-order transition from the liquid to the hexatic and a continuous transition from the the hexatic to the solid.