DY 22: Statistical Physics (general)

Time: Wednesday 15:00–18:15 Location: ZEU 160

DY 22.1 Wed 15:00 ZEU 160

Hamiltonian adaptive resolution simulations of soft matter — •Raffaello Potestio — Max Planck Institute for Polymer Research, Mainz

Many phenomena occurring in soft matter, from the interaction of biomolecules to the self-assembly of biological as well as artificial nanocomposites, cover a broad range of length and time scales. Being hardly amenable with a fully-atomistic approach, these systems are usually addressed with multiscale simulation methods, aimed at building computationally efficient coarse-grained models that, in many cases, suffer the lack of important chemical details. To circumvent this problem, adaptive dual-resolution schemes have been developed to concurrently use different levels of resolution in different regions of the same system, yet allowing molecules to freely diffuse across the simulation domain. Here a method is presented, the Hamiltonian Adaptive Resolution Simulation (H-AdResS) scheme, which, in contrast to previous approaches, is built in terms of a Hamiltonian function; this makes it possible to formulate a solid statistical physics theory of dual-resolution systems and, as a consequence, it allows one to use the preferred statistical ensemble as well as the simulation algorithm. Applications of H-AdResS will be discussed, such as microcanonical simulations of simple molecular fluids and Monte Carlo simulations of mixtures.

DY 22.2 Wed 15:15 ZEU 160

parQ - Infinite Temperature Transition Matrix Monte Carlo in the Canonical and Grand Canonical Ensemble — •René Haber and Karl Heinz Hoffmann — Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany

We investigate properties of our transition matrix Monte Carlo method par$Q$[1] in the canonical and grand canonical ensemble. It estimates the transition probabilities at infinite temperature in a given macrostate range by counting all proposed transitions during a simulation. At the end of the simulation the eigenvector corresponding to the eigenvalue 1 is calculated, which can be identified as the density of states. The method is easily parallelizable and can be combined with different sampling schemes like standard Metropolis sampling, Wang-Landau sampling as well as transition matrix Monte Carlo. The influence of different sampling schemes and different eigenvector solving algorithms is presented.

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

DY 22.3 Wed 15:30 ZEU 160

Dynamics in Stochastic Optimization: Combining Stochastic Tunneling and Energy Landscape Paving — •Kay Hamacher — Depts. of Physics, Computer Science, and Biology, TU Darmstadt

Heuristic optimization schemes such as simulated annealing, genetic algorithms, or extremal optimization play a most prominent role in global optimization. The performance of these algorithms and their respective sampling behavior during the search process are themselves interesting problems - in particular from the viewpoint of dynamical systems theory and statistical mechanics.

Here, we show that a combination of two approaches * namely Energy Landscape Paving (ELP) and Stochastic Tunneling (STUN) * can overcome known problems of other Metropolis-sampling-based procedures. We show on grounds of non-equilibrium statistical mechanics and empirical evidence on the synergistic advantages of this combined approach and discuss simulations for a complex optimization problem.

Reference: [1] K. Hamacher. A New Hybrid Metaheuristic - Combining Stochastic Tunneling and Energy Landscape Paving, 8th International Workshop on Hybrid Metaheuristics (HM2013), Lecture Notes in Computer Science (LNCS 7919), pp. 107-117, 2013.

DY 22.4 Wed 15:45 ZEU 160

Semiclassical Spectral Function for Matter Waves in Random Potentials — •Martin-Isbjörn Trappe[1] and Cord Axel Müller[2] — [1]Centre for Quantum Technologies, National University of Singapore — [2]Department of Physics, University of Konstanz, Germany

We derive the first order quantum corrections of the spectral function for matter waves with quadratic dispersion in correlated random potentials using the Wigner function. The spectral density is in particular relevant for the investigation of Anderson localization in laser speckle potentials. The Wigner function approach allows for a systematic semiclassical expansion of the spectral function to arbitrary orders of Planck's constant. We especially consider Gaussian as well as speckle random processes and compare to numerical results. For the case of speckle potentials we present a closed expression for the generating functional.

DY 22.5 Wed 16:00 ZEU 160

Signatures of Symmetry Classes in the Many-Body Transition Amplitude in Fock Space — •Thomas Engl, Juan Diego Urbina, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, D-93040 Regensburg, Germany

The Bohigas-Giannoni-Schmit (BGS) conjecture states that the energy levels of a single-particle quantum system with classically chaotic counterpart shows the same statistics as that of a Gaussian random matrix satisfying certain symmetries. Semiclassical methods based on the van Vleck-Gutzwiller propagator are able to capture quantum interference effects, and provide a natural route to confirm this conjecture [1]. Therefore, universal effects depending merely on the symmetry class of the described system can be semiclassically understood.

Recently, a semiclassical propagator in Fock space has been derived [2] that accounts for quantum interference in bosonic many body systems. Here we extend this work to interacting fermionic systems and investigate the transition amplitude in Fock space as an indicator of different universality classes. Amongst others, we find an analog of antilocalization for the Gaussian symplectic ensemble corresponding to time reversal invariant spin-1/2 systems.

[1] S. Müller, S. Heusler, A. Altland, P. Braun and F. Haake, New Journal of Physics **11** 103025 (2009)
[2] T. as Engl, J. Dujardin, A. Argüelles, P. Schlagheck, K. Richter and J. D. Urbina, arXiv:1306.3169

DY 22.6 Wed 16:15 ZEU 160

Nonlinear response of a linear chain to weak driving — •Colm Mulhern — Max Planck Institute for the Physics of Complex Systems, Germany

We study the escape of a chain of coupled units over the barrier of a metastable potential. It is demonstrated that a very weak external driving field with suitably chosen frequency suffices to accomplish speedy escape. The latter requires the passage through a transition state the formation of which is triggered by permanent feeding of energy from a phonon background into humps of localised energy and elastic interaction of the arising breather solutions. In fact, cooperativity between the units of the chain entailing coordinated energy transfer is shown to be crucial for enhancing the rate of escape in an extremely effective and low-energy cost way where the effect of entropic localisation and breather coalescence conspire.

15 min break

DY 22.7 Wed 16:45 ZEU 160

From the nonstationarity of the hysteresis memory to a nonstationary response — •Sven Schubert and Günter Radons — TU Chemnitz, 09107 Chemnitz, Germany

A certain memory causes the dependence on the history of an external field and the multistability which are typical features of systems with hysteresis. We consider the number of values N_t stored by hysteresis models, like the Preisach model and the zero-temperature random field Ising model, which are subjected to uncorrelated stationary driving.

The time-dependent probability distribution $P_t(N)$ of the memory length is derived using methods known from record statistics. It is shown that the memory length is on average diverging with time t. Thus, the hysteresis memory caused by uncorrelated stationary noise becomes a nonstationary process, even in the long-time limit.

The nonstationarity of the memory is reflected, for instance, in possible long-time tails in the autocovariance of the stationary response of the Preisach model [1]. Furthermore, the hysteretic response can become a nonstationary process with stationary increments leading on to $1/f$-noise. We elucidate this mechanism using an example of the symmetric Preisach model and present rigorous results on the power spectral density of the model's response to uncorrelated driving.

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

DY 22.8 Wed 17:00 ZEU 160

Density functional theory for elongated polyhedra — •Matthieu Marechal and Klaus Mecke — Friedrich-Alexander-Universität Erlangen-Nürnberg

Due to recent advances in synthesis of nanoparticles and colloids, many-particle system of polyhedra are readily available for experiments. This has spurred a host of many-particle simulation studies on polyhedra. More recently, the lack of theoretical tools to study these system was amended by proposing a density functional theory (DFT) for polyhedra using the frame work of fundamental measure theory.

In this talk, the application of DFT to elongated polyhedra will be discussed. Recent advancements in the DFT of long rods allow us to consider nematic and smectic liquid crystals in addition to the isotropic phase. We will first consider these phases for triangular prisms that are elongated along their rotation axis. We validate the DFT approach by comparing to Monte Carlo computer simulations and we calculate the liquid crystal phase diagram.

Colloidal prisms with arbitrarily shaped bases have been synthesized using nanolithography; our DFT approach allows to explore the enormous ensuing shape parameter space. We focus on smectic phases and determine which shapes show a global tilt between the particle direction and the layer normal ('smectic C') or a splitting of the layer into two layers (bilayer smectic). We hope our results motivate further experiments on colloidal smectics.

DY 22.9 Wed 17:15 ZEU 160

2D Melting in General: Solid/hexatic/liquid Phase Transitions in Soft Spheres using Event-Chain Monte Carlo — •Sebastian C Kapfer, Manon Michel, and Werner Krauth — LPS, Ecole normale supérieure, Paris, France

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 unbindung and a conventional first-order liquid/solid transition. For hard disks, a rather unexpected hybrid transition has recently been found with both a first-order transition and an intermediate hexatic phase [1], while magnetic colloid experiments support the KTHNY scenario [2]. To resolve this discrepancy, we here address the melting problem for soft interaction potentials, in particular the nature of the liquid/hexatic and hexatic/solid transitions, and the defects driving melting. Simulations were effected by a new rejection-free irreversible Monte Carlo algorithm generalizing event-chain Monte Carlo to soft arbitrary pair potentials. In addition to fast equilibration, this algorithm allows to deduce pressure in the NVT ensemble without any additional computations [3].

[1] E. P. Bernard, W. Krauth, Phys. Rev. Lett. 107, 155704 (2011). [2] P. Keim et al. Phys. Rev. Lett. 92, 215504 (2004). [3] M. Michel et al., preprint at arXiv:1309.7748.

DY 22.10 Wed 17:30 ZEU 160

Ising Kagome Paramagnet is a Mean-Field system — •Taras Yavors'kii — AMRC, Department of Mathematics and Physics, Coventry University, CV1 5FB, England

Antiferromagnetic nearest-neighbor Ising model on a geometrically frustrated two-dimensional kagome lattice does not order down to $T = 0$ [1]. Using Monte Carlo simulations on graphics processing units (GPUs) as a tool, I show that statistical physics properties of the model, including pair correlation function and specific heat, are well described by the variational single-particle mean-field theory [2] (MFT) ansatz at *all* $T \geq 0$, provided the MFT temperature scale Θ, where $\Theta_c < \Theta < \infty$, is mapped onto the physical temperature scale $0 \leq T < \infty$ by considering Θ as a suitable function of T. The model is thus completely "transparent" to the paramagnetic MFT treatment deep below the MFT critical temperature $\Theta_c > 0$, making MFT a simple and powerful tool for the study of perturbations at low T.

[1] K. Kanô and S. Naya, *Prog. Theor. Phys.* **10** 158 (1953)

[2] P. M. Chaikin and T. C. Lubensky, *Principles of Condensed Matter Physics* (Cambridge University Press, Cambridge, UK, 1995)

DY 22.11 Wed 17:45 ZEU 160

A Maxwell's demon action on a tape with energy exchange — •Johannes Hoppenau — Carl-von-Ossietzky Universität Oldenburg, 26111 Oldenburg, Germany

Currently, in statistical physics, models that incorporate information processing are of lively interest. Several of these models consider an information carrying tape. Typically, it is assumed that no energy is needed to store information on this tape. We investigate how things change, if this assumption is relaxed. Therefore, we propose a model of a tape, where the information is encoded in a two-level systems, via its energystates. In this model energy is needed to write information. Our focus is on the efficiency of devices that are coupled to such a tape. We derive an upper bound for the efficiency, which is more restrictive than the Carnot bound. This bound holds whether or not the model contain feedback.

DY 22.12 Wed 18:00 ZEU 160

Approximative counting of Manifold Triangulations — •Benedikt Krüger and Klaus Mecke — Institut für Theoretische Physik, FAU Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Each topological manifold in 2d and 3d permits a finite number of non-equivalent discretisations into combinatorial manifolds or triangulations with given number of vertices or maximal simplices. This number of distinct triangulations is important for questions arising in topology, geometry and physics. e.g. in quantum gravity [1].

Until now the best method for the counting of combinatorial manifolds was the isomorphism free enumeration of all possible triangulations which succeeded for vertex numbers below about 15 [2]. We use Monte-Carlo algorithms for estimating the number of triangulations of two- and three-dimensional manifolds and show that we are able to increase the known regime of triangulation counts by one magnitude. We give numerical evidence that the number of surface triangulations scales exponentially with the vertex number and that the rate of growth depends linearly on the genus of the surface.

[1] J. Ambjørn, J. Jurkiewicz, and R. Loll, Phys. Rev. D 72, 064014 (2005)

[2] T. Sulanke and F. H. Lutz, Eur. J. Comb. 30, 1965 (2009)