DY 6: Statistical Physics: General I

Time: Monday 10:00–13:00 Location: ZEU 160

DY 6.1 Mon 10:00 ZEU 160

Noether's theorem in statistical mechanics — •Sophie Hermann and Matthias Schmidt — Universität Bayreuth, Bayreuth, Deutschland

Noether's Theorem is familiar to most physicists due its fundamental role in linking the existence of conservation laws to the underlying symmetries of a physical system. Typically the systems are described in the particle-based context of classical mechanics or on the basis of field theory. We apply Noether's calculus of invariant variations to thermal systems, where fluctuations are paramount and one aims for a statistical mechanical description, both in and out of equilibrium. Generating functionals, such as the free energy, yield mechanical laws under continuous translational and rotational symmetry operations. The resulting global theorems express vanishing of total internal and total external forces and torques. Local sum rules interrelate density correlators, as well as static and time direct correlation functions via infinite hierarchies, including memory. We demonstrate that this approach is consistent with the earlier work in equilibrium, and that it enables one to go, with relative ease, beyond the sum rules that these authors formulated. For anisotropic particles, systematic coupling of orbital and spin motion is identified. The theory allows to shed new light on the spatio-temporal coupling of correlations in complex systems. We present novel exact and nontrivial identities that apply to time-dependent problems and driven and active fluids.

DY 6.2 Mon 10:15 ZEU 160

Mean-field brittle yielding of amorphous solids — •Jack T. Parley[1] and Peter Sollich[1,2] — [1]Institut für Theoretische Physik, University of Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany — [2]Department of Mathematics, King's College London, London WC2R 2LS, UK

We study the brittle yielding of athermal amorphous solids within the celebrated Hébraud-Lequeux mean-field elastoplastic model, which incorporates the sign-varying nature of Eshelby interactions as a Gaussian mechanical noise. As in finite-dimensional particle simulations, we find a critical value of the initial disorder, below which yielding in the limit of quasistatic shear becomes a discontinuous non-equilibrium transition. We find evidence that in this limit yielding cannot be described as a spinodal instability, in contrast to the behaviour found in driven random magnets or depinning-like models. At small but finite shear rates, we show that the tail exponents characterising the decay of the plastic yield rate function on either side of its peak at the transition are related to the athermal aging exponents. We finally derive analytically the scaling with shear rate of the peak susceptibility at the random critical point, and discuss the connection to avalanches in finite-size systems.

DY 6.3 Mon 10:30 ZEU 160

Bringing the power of Monte Carlo methods to long-range-interacting molecular systems — •Philipp Höllmer[1], A. C. Maggs[2], and Werner Krauth[3] — [1]University of Bonn, Germany — [2]ESPCI Paris, France — [3]École normale supérieure de Paris, France

Molecular simulations are widespread in molecular sciences to study, e.g., protein folding. Here, chemical systems are modeled empirically by a set of atomic positions with parameterized interaction potentials. Nowadays, molecular-dynamics (MD) simulations are predominantly used to study long-range-interacting molecular systems because of their superior computational complexities and Newtonian dynamics when compared to traditional Markov-chain Monte Carlo (MCMC) simulations. We argue that both disadvantages of traditional reversible MCMC are overcome by event-chain Monte Carlo (ECMC), which is a family of non-reversible MCMC methods.

In this talk, we will explore how ECMC samples the equilibrium Boltzmann distribution exactly, although it uses non-equilibrium dynamics and never computes the total system potential. We will discuss how ECMC's sole restriction of the global-balance condition yields a great freedom to implement quickly decorrelating dynamics beyond Newtonian's dynamics of MD. Finally, we will demonstrate $\mathcal{O}(N \log N)$ scaling for ECMC's decorrelation of an N-body system of a commonly used long-range-interacting water model. This matches the performance of MD without ever discretizing time or space.

DY 6.4 Mon 10:45 ZEU 160

Virial coefficients of hard, anisotropic particles in two- to four-dimensional Euclidean spaces — •Markus Kulossa, Daniel Weidig, and Joachim Wagner — Institut für Chemie, Universität Rostock, 18051 Rostock, Germany

We compare virial coefficients up to order eight for anisotropic, hard particles in two- to four-dimensional Euclidean spaces in dependence on their aspect ratio. The virial coefficients of both, convex shapes such as stadia, spherocylinders and hyperspherocylinders and concave shapes such as dumbbells in two to four dimensions are analyzed. Since the second virial coefficient of hard objects equals their mutual excluded D-dimensional volume per particle, analytically obtained expressions for the second virial coefficients serve as a test for orientation-dependent overlap algorithms. In first approximation, a nearly universal dependence of reduced virial coefficients on the excess part of the mutual excluded volume is observed for third and higher order virial coefficients.

DY 6.5 Mon 11:00 ZEU 160

Geometric Bounds on the Power of Adiabatic Thermal Machines — •Joshua Eglinton[1,2] and Kay Brandner[1,2] — [1]School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, United Kingdom — [2]Centre for the Mathematical and Theoretical Physics of Quantum Non-equilibrium Systems, University of Nottingham, Nottingham NG7 2RD, United Kingdom

The laws of thermodynamics put fundamental bounds on the efficiencies of thermal machines. These Carnot bounds can typically be attained only if the machine is operated quasi-statically, which leads to vanishing power output. We present a new family of power-efficiency trade-off relations that imply a quadratic decay of power at Carnot efficiency, for devices operating between two fixed temperatures. Notably, these relations depend only on geometric quantities such as the thermodynamic length of the driving cycle and hold for essentially any thermodynamically consistent micro-dynamics such as classical Markov-jump processes, adiabatic Lindblad dynamics or coherent transport. This analysis is based on a new general scaling argument, with which we show that the efficiency of such devices reaches the Carnot bound only if heat-leaks between the baths can be fully suppressed. Furthermore, we find that their power is in fact determined by second-order terms in the temperature difference between the two baths, which are neglected in standard linear-response theory.

[1] - J. Eglinton and K. Brandner, Phys. Rev. E 105, L052102 (2022)

DY 6.6 Mon 11:15 ZEU 160

Hard rods on a 2D lattice system — •Michael Zimmermann — Universität Tübingen, Tübingen, Deutschland

An exact solution for the equilibrium density for a hard rod system on a 1D continuous system was found by Percus [1]. For lattice systems of hard rods, Lafuente and Cuesta established a method based on Rosenfeld's fundamental measure theory to find the exact solution in 1D and to extrapolate from this result to a density functional in higher dimensions [2,3]. But already in 2D theoretical properties differ from respective simulation results [4], such as the onset of demixing between rods of different orientation. In this talk we will discuss some possible extensions of the Lafuente-Cuesta functional for improving the excess free energy functional and for better approximations of density distributions in 2D hard rod lattice systems.

[1] Percus J. K. 1976 J. Stat. Phys. 15 505*11 [2] Rosenfeld Y. 1989 Phys. Rev. Lett. 63 980*3 [3] Lafuente L. and Cuesta J.A. 2002 J. Phys.: Condens. Matter 14 12079 [4] Oettel M., Klopotek M. et al 2016 J. Chem. Phys. 145 074902

15 min. break

DY 6.7 Mon 11:45 ZEU 160

Mean first-passage times of continuous-time random walkers determined through Wiener-Hopf integral equations — •Marcus Dahlenburg[1,2] and Gianni Pagnini[1,3] — [1]BCAM-Basque Center for Applied Mathematics, Alameda de Mazarredo 14, 48009 Bilbao, Basque Country, Spain — [2]Institute for Physics & Astronomy, University of Potsdam, 14476 Potsdam, Germany — [3]Ikerbasque-Basque Foundation for Science, Plaza Euskadi 5, 48009 Bilbao, Basque

Country, Spain

Asymmetric continuous-time random walks in continuous-space characterised by waiting-times with finite mean and by jump-amplitudes with both finite mean and finite variance are governed by an advection-diffusion equations in the asymptotic limit. The mean first-passage time (MFPT) of such an advective-diffusive system on a halfline results to be finite when the advecting drift is in the direction of the boundary. In our investigation we derive an inhomogeneous Wiener-Hopf integral equation that allows to avoids approximated results in the asymptotic limits and leads indeed to the exact determination of the MFPT. This quantity depends on the average of the waiting-times only but it conserves the information about the whole distribution of the jump-amplitudes. Through the case study of asymmetric double-exponential distributions of the jump-amplitudes one may identifies a length-scale, that defines the transition from starting points near the boundary to starting points far-away from the boundary where the MFPT loses the information about the exact shape of the jump-amplitudes' distribution and only conserves their mean.

DY 6.8 Mon 12:00 ZEU 160

A combinatorial approach to the many-body density of levels and the Bethe approximation — •Carolyn Echter, Georg Maier, Juan-Diego Urbina, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Regensburg, Germany

The Bethe formula, originally derived in [1] to estimate the density of levels of heavy nuclei, has become a widely used approximation for the many-body density of levels of a non-interacting fermionic system, appropriate for large numbers of particles and energies in a system-dependent range. Notably, in the case of equally spaced single-particle energy levels, it coincides with the asymptotic result for the number of unrestricted partitions of an integer known from analytic number theory [2]. An explanation is suggested by the combinatorics of distributing integer amounts of energy to particles obeying given statistics. We present a combinatorial derivation of the exact many-body density of levels for various particle statistics in the case of a constant single-particle density of states, thereby adding to existing discussions [3,4] and explaining the asymptotic agreement of Bethe's approximation with number theoretical partition functions. We compare numerically with semiclassical results and make suggestions towards a bosonic analogue of the Bethe formula based on our observations.

[1] H. A. Bethe, Phys. Rev. 50, 332-41 (1936). [2] G. H. Hardy, S. Ramanujan, Proc. London Math. Soc. (2) 17, 75-115 (1918). [3] F. C. Auluck, D. S. Kothari, Math. Proc. Camb. Philos. Soc. 42, 272-77 (1946). [4] A. Comtet, P. Leboeuf, S. N. Majumdar, Phy. Rev. Lett. 98, 070404 (2007).

DY 6.9 Mon 12:15 ZEU 160

Integral Equations in Statistical Mechanics: A Size-effect Study — •Jose Mauricio Sevilla Moreno and Robinson Cortes-Huerto — Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Integral equations (IE) are in the core of statistical mechanics of liquids as they connect the local structure with thermodynamic properties as compressibility, activity coefficients and excess entropy. IE are normally defined in the grand canonical ensemble and calculated in the thermodynamic limit (TL). By contrast, computer simulations are performed with finite-size systems and mimic the TL using periodic boundary conditions (PBC). This proceeding introduces several finite-size contributions whose effects must be identified and corrected in order to approximate the simulation results to the TL. In this talk, we present a generic method to compute IE from molecular dynamics simulations. In our approach, we define finite-size IE, integrating them in Fourier space to trivially introduce PBC. This procedure allows us to identify and isolate ensemble, finite-volume domains and PBC effects and accurately obtain the corresponding thermodynamic quantities in the TL or artificially for any finite size system. To validate our method, we compute isothermal compressibilities, chemical potentials and excess entropies of simple liquids and liquid mixtures, including water and aqueous alcohol solutions, showing good agreement with results available in the literature.

DY 6.10 Mon 12:30 ZEU 160

A Multiscale Approach for Large-Scale Proton Dynamics Simulations — •Christian Dressler[1] and Daniel Sebastiani[2] — [1]TU Ilmenau, Institute of Physics, Theoretical Solid State Physics — [2]MLU Halle-Wittenberg, Institute of Chemistry, Theoretical Chemistry

We present a multiscale simulation approach for the calculation of proton diffusion/conduction in disordered organic and inorganic materials. We combine quantum chemical calculations for elementary reactions between the ions and surrounding molecules with molecular dynamics simulations for the incorporation of local dynamical heterogeneities at the nanometer/nanosecond scale. Data from both levels are integrated in a stochastic propagation scheme (Monte Carlo or Markov matrix approach) for the simulation of proton transfer at much larger time and length scales. The approach allows for an atom-level resolution of ion dynamics with quantum chemical accuracy but with final length- and time-scales of micrometers and milliseconds. As a proof-of-principle simulation, we have computed the explicit dynamics of a non-equilibrium process in an 8 μm CsH_2PO_4 system during 5 ms. Finally, we demonstrate the application potential of the scheme by computing the proton conductivity of a nanostructured CsH_2PO_4 fuel cell membrane with respect to the porosity.

DY 6.11 Mon 12:45 ZEU 160

Population Annealing and the Role of Resampling in Population Annealing — •Denis Gessert[1,2], Martin Weigel[3], and Wolfhard Janke[1] — [1]Institut für Theoretische Physik, Leipzig University, Postfach 100920, D-04009 Leipzig, Germany — [2]Centre for Fluid and Complex Systems, Coventry University, Coventry CV1 5FB, United Kingdom — [3]Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

Studying equilibrium properties of thermodynamic systems with rough free-energy landscapes particularly challenges standard Markov chain Monte Carlo techniques such as the Metropolis algorithm. Sampling can be improved by using generalized ensemble methods, one of which is Population Annealing (PA). Although PA is not expected to outperform its contenders in terms of time complexity, it is particularly well suited for parallel execution with no theoretical limit on the level of parallelism, which makes it a viable option on modern HPC.

In PA a population of replicas is collectively cooled down. At each temperature a population control step is carried out before applying some replica-independent update moves. This population control is realized by means of resampling. Here, we compare various different resampling methods and their performance in PA applications. Using the $d = 2$ Ising model as a benchmark system, we identify two resampling methods that appear preferable over the widely used multinomial resampling. Further, we point out when different resampling choices affect the statistical quality of the simulation outcome and obtain some model-independent guiding principles for the choice of PA parameters.