DY 5: Statistical Physics: General

Time: Monday 9:30–11:15 Location: H47

DY 5.1 Mon 9:30 H47

The scaling behaviour of localised and extended states in one-dimensional tight-binding models with disorder — •Luca Schaefer and Barbara Drossel — Technische Universität Darmstadt, Hochschulstraße 6, 64289 Darmstadt

We investigate two one-dimensional tight-binding models with disorder that have extended states at zero energy. We use the eigenmodes of the Hamiltonian and the associated participation ratios, and the transfer-matrix method to determine the localisation length. The first model has no on-site disorder, but random couplings. While the participation ratio remains finite at zero energy, the localisation length diverges logarithmically as the energy goes to zero. We provide an intuitive derivation of this logarithmic divergence based on the weak coupling of the two sublattices. The second model has a conserved quantity as the row sums of the Hamiltonian are zero. This model can be represented as a harmonic chain with random couplings, or as a diffusion model on a lattice with random links. We find, in agreement with existing analytical calculations, that the number of system-spanning eigenmodes increases proportionally to the square root of the system size, and we related this power law to other power laws that characterise the scaling behaviour of the eigenmodes, the participation ratio, the localisation length, and their dependence on energy and system size. When disorder is so strong that the smallest hopping terms can be arbitrarily close to zero, all these power laws change, and we show a crossover between the two scaling regimes. All these results are explained by intuitive arguments based on scaling.

DY 5.2 Mon 9:45 H47

How hidden free energy landscapes imprint on the time-ordering of observed states — •Francesco Malcangi and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

Single molecule experiments, such as FRET, Plasmon Ruler, or optical tweezers, probe low (often one-) dimensional projections of high dimensional dynamics. Unless the unobserved, hidden degrees of freedom relax much faster than the observable, the projection induces memory effects. By accessing the information encoded in the time-ordering of projected states, we show in our work that opportunely chosen functionals of observed paths, in particular their fluctuations and correlations, may be used to infer the presence of hidden free-energy barriers, multiple pathways, and even irreversible drifts. These hidden features are found to display common manifestations upon projection, which together with the comparison with manifestly Markovian dynamics in the free energy landscape may be used as a diagnostic tool. We demonstrate our findings with illustrative examples.

DY 5.3 Mon 10:00 H47

Long-term behavior of master equations on a countable system — •Bernd Michael Fernengel[1], Thilo Gross[1], and Wolfram Just[2] — [1]HIFMB, Oldenburg, Germany — [2]University of Rostock, Rostock, Germany

Master equations play a crucial role in natural science, as they describe the time evolution of probability distributions of all systems that can be modeled as directed, weighted graphs. Despite their essential role, computing a solution is often avoided and authors refer to numerical methods or approximation techniques instead.

We present both a mathematically sound framework for master equations on a discrete, countable configuration space as well as sufficient conditions the generator of the master equation must have for the time limit t -> infinity to converge, which is not guaranteed on an infinite dimensional space.

We discuss the assumptions for the possibility of interchanging the thermodynamic limit and the time limit. This makes it possible to obtain the long-term behavior of an infinite system from a thermodynamic limit of stationary solutions of corresponding finite subnetworks.

Our method is demonstrated by a few examples of master equations on linear, infinitely long chains, with one- and two open ends.

DY 5.4 Mon 10:15 H47

Density Fluctuations, Solvation Thermodynamics and Coexistence Curves in Grand Canonical Molecular Dynamics Simulations — •Mauricio Sevilla, Luis A. Baptista, Kurt Kremer, and Robinson Cortes-Huerto — Max Planck Institute for Polymer Research

The physics of externally driven systems is a challenge as the complexity of the amount of effects involved, yet crucial to be understood as it is present in many biological systems. Aiming to build a computational method to deal with such situations, it is first needed to reproduce correctly the equilibrium statistics of open systems. However, open-boundary computational methods are scarce and often do not satisfy all the conditions imposed by reality. The system of interest (SoI) must be at thermodynamic and chemical equilibrium with an infinite reservoir of particles. The fluctuations of the SoI in equilibrium should sample the grand canonical ensemble. The local solvation thermodynamics, extremely sensitive to finite-size effects due to particle depletion, should be correctly described. The method should be robust enough to deal with phase transitions and coexistence conditions that might occur in the SoI. In this context, the adaptive resolution method (AdResS), where the system's atomistic and ideal gas representations coexist at constant thermodynamic and chemical equilibrium, emerges as a promising alternative. Indeed, in this talk, we demonstrate with prototypical liquid systems that AdResS, coupled with particle insertion/deletion steps, satisfies all these requirements, and it is thus a suitable method to perform simulations of open systems.

DY 5.5 Mon 10:30 H47

Optimal control of fluid transitions in a Lennard-Jones like system — •William D. Pineros and Etienne Fodor — Department of Physics and Material Science, University of Luxembourg, 162a, avenue de la Faïencerie, L1511, Luxembourg

We study optimal control transitions in a system of Lennard-jones like fluid via a linear-response framework whose solutions correspond to minimum dissipation protocols in a thermodynamic space. In particular, we investigate fluid-fluid transitions via changes in particle size and attraction strength both in the homogenous and phase separated state. We compute the underlying friction tensor, representing the ease of parameter change in this space, directly from simulations and compare against an analytical approximation for low density fluids at the continuum level.

DY 5.6 Mon 10:45 H47

Noether-constrained correlations and hyperforces in equilibrium liquids — •Sophie Hermann[1,2], Silas Robitschko[1], Florian Sammüller[1], and Matthias Schmidt[1] — [1]Universität Bayreuth, Bayreuth, Germany — [2]Sorbonne Université/CNRS, Paris, France

Noether's calculus of invariant variations in statistical mechanics yields exact identities ("sum rules") from functional symmetries. The invariance of spatial transformation of the underlying classical many-body Hamiltonian at first order in the transformation field Noether's theorem yields the local force balance. At second order three distinct two-body correlation functions emerge, namely the standard two-body density, the localized force-force correlation function, and the localized force gradient. An exact Noether sum rule interrelates these correlators. More generally exploiting invariance of a thermally averaged classical phase space functions results in hyperforce sum rules. These relate the mean gradient of a phase-space function to its negative mean product with the total force. As applications we investigate via computer simulations (including Lennard-Jones liquids, monatomic water and a colloidal gel former) the emerging one-body force fluctuation profiles in bulk and confined liquids. These local correlators quantify spatially inhomogeneous self-organization, demonstrate their fundamental role in the characterization of spatial structure and their measurement allows for the development of stringent convergence tests and enhanced sampling schemes in complex systems.

DY 5.7 Mon 11:00 H47

Hybrid particle-phase field model and renormalized surface tension in dilute suspensions of nanoparticles — •Alexandra Hardy, Abdallah Daddi-Moussa-Ider, and Elsen Tjhung — The Open University, Milton Keynes, UK

We present a two-phase field model and a hybrid particle-phase field model to simulate dilute colloidal sedimentation and flotation near a liquid-gas interface (or fluid-fluid interface in general). Both models

are coupled to the incompressible Stokes equation, which is solved numerically using a combination of sine and regular Fourier transforms to account for the no-slip boundary conditions at the boundaries. The continuum two-phase field model allows us to analytically solve the equilibrium interfacial profile using a perturbative approach, demonstrating excellent agreement with numerical simulations. Notably, we show that strong coupling to particle dynamics can significantly alter the liquid-gas interface, thereby modifying the liquid-gas interfacial tension. In particular, we show that the renormalized surface tension is monotonically decreasing with increasing colloidal particle concentration and decreasing buoyant mass.