DY 30: Statistical Physics far from Thermal Equilibrium

Time: Wednesday 10:00–12:45 Location: H6

Invited Talk DY 30.1 Wed 10:00 H6

Fluctuations and responses in nonequilibrium fluids — •Matthias Krüger — Institut für Theoretische Physik, Georg-August-Universität Göttingen

Understanding systems far from equilibrium is of fundamental and technological interest. The linear response of systems mildly perturbed from equilibrium can be understood in terms of the well known fluctuation-dissipation-theorem (FDT). Further away from equilibrium, the situation is generally less clear, and is the topic of manifold ongoing investigations.

We derive a path-integral version of nonlinear response theory, which can be considered an extension of the FDT to nonlinear responses, and discuss the fundamental properties of such extensions in relation to the FDT itself, and also test it experimentally in a colloidal model system.

These path integral techniques can also be used to derive Langevin-descriptions for nonlinear fluids, necessary for understanding the motion of (driven) probe particles in (nonlinear) viscoelastic surroundings; Indeed, due to the nonlinear responses of viscoelastic solvents (such as shear thinning behavior), a driven colloidal particle can display pronounced nonequilibrium fluctuations already at slow driving speeds, as will be demonstrated using recent experimental data.

DY 30.2 Wed 10:30 H6

Transmission from reverse reaction coordinate mappings — •Niklas Martensen and Gernot Schaller — Institut für Theoretische Physik, Hardenbergstr. 36, Technische Universität Berlin, D-10623 Berlin, Germany

We point out that the transport properties of non-interacting fermionic chains that are tunnel-coupled to two reservoirs at their ends can be mapped to those of a single quantum dot that is tunnel-coupled to two transformed reservoirs. The parameters of the chain are mapped to additional structure in the spectral densities of the transformed reservoirs. For example, this enables the calculation of the transmission of quantum dot chains by evaluating the known transmission of a single quantum dot together with structured spectral densities. We exemplify this analytically for short chains, which allows to optimize the transmission. Tuning of the transmission allows to reach a non-Markovian transport regime that violates the thermodynamic uncertainty relation. In addition, we also demonstrate that the mapping can be performed numerically by computing the transmission of a Su-Schrieffer-Heeger chain.

[1] A. Nazir and G. Schaller, *The reaction coordinate mapping in quantum thermodynamics*, as a chapter of F. Binder, L. A. Correa, C. Gogolin, J. Anders, and G. Adesso (eds.), Thermodynamics in the quantum regime - Recent Progress and Outlook (Springer International Publishing), arXiv:1805.08307.

[2] N. Martensen and G. Schaller, *Transmission from reverse reaction coordinate mappings*, arXiv:1809.10529.

DY 30.3 Wed 10:45 H6

Thermoelectric performance of topological boundary modes — •Sina Böhling[1], Georg Engelhardt[2], Gloria Platero[3], and Gernot Schaller[1] — [1]Technische Universität Berlin, Berlin, Germany — [2]Beijing Computational Science Research Center, Beijing, People's Republic of China — [3]Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid, Spain

We investigate quantum transport and thermoelectrical properties of a finite-size Su-Schrieffer-Heeger model, a paradigmatic model for a one-dimensional topological insulator, which displays topologically protected edge states. By coupling the model to two fermionic reservoirs at its ends, we can explore the non-equilibrium dynamics of the system. Investigating the energy-resolved transmission and the current, we find that these observables can be used to detect the topologically non-trivial phase.

In addition, we point out that the edge states can be exploited to design a refrigerator driven by chemical work or a heat engine driven by a thermal gradient, respectively. These thermal devices do not require asymmetric couplings and are topologically protected against symmetry-preserving perturbations. Their maximum efficiencies significantly exceed that of a single quantum dot device at comparable coupling strengths.

[1] S. Böhling, G. Engelhardt, G. Platero, and G. Schaller, *Thermoelectric performance of topological boundary modes*, Phys. Rev. B **98**, 035132 (2018)

DY 30.4 Wed 11:00 H6

The Quantum Otto Engine in Finite Time: Dynamics, Thermodynamics and Coherence — Michael Wiedmann, •Jürgen T. Stockburger, and Joachim Ankerhold — Ulm University, Institute for Complex Quantum Systems

We perform complete, exact dynamical simulations of the quantum Otto engine in terms of the full, interacting dynamics of the work medium and its two thermal reservoirs. In this context, the Otto cycle is defined by externally modulating the oscillation frequency of the work medium ("piston") and the coupling constants to the reservoirs ("valves"). We find that the work expended in operating the "valves" is far from negligible in this engine. Moreover, the system dynamics in cyclic operation displays non-thermal effects (squeezing, coherence), which should be taken into account in the finite-time thermodynamics of the Otto cycle.

15 min. break

DY 30.5 Wed 11:30 H6

Violation of Jarzynski Equality using catalysts — •Paul Boes[1], Rodrigo Gallego[1], Henrik Wilming[2], Nelly Ng[1], Markus Müller[3,4], and Jens Eisert[1] — [1]Freie Universität Berlin, Deutschland — [2]ETH Zürich, Schweiz — [3]IQOQI Wien, Österreich — [4]Perimeter Institute, Kanada

Fluctuation theorems are concerned with the probability distributions of work in a scenario where we measure the energy of a system in a Gibbs state, evolve it unitarily and then measure the energy again. In this setting, the second law states that it is impossible to extract work on average, while fluctuation theorems impose further constraints on the fluctuations of work. In this work, we study a generalization of this typical setup that additionally allows for the use of catalytic systems. In this setting, the usual second law continues to hold, however, fluctuation theorems can be violated. In particular, we show that it is possible to extract, for large systems, a finite amount of work per particle with a finite probability. This can be recast as the statement that the Jarzynski equality can be violated by an amount which diverges exponentially with the system size, at the cost of having to use increasingly large catalytic systems.

DY 30.6 Wed 11:45 H6

Field theory for interacting Brownian particles — •Rohit Jain[1] and Matthias Krüger[2] — [1]Institut für Theoretische Physik, 37077 Göttingen, Germany — [2]Institut für Theoretische Physik, 37077 Göttingen, Germany

We derive a field theory for interacting Brownian particles starting from the stochastic equation for the density operator [1], using different approximations [2]. This field theory, among other things, can be used to analyze stresses and forces in non-equilibrium scenarios [3]. We discuss and analyze several applications. For instance, with this approach, we calculate the time-dependent two-point correlation functions. We also discuss the relation of this approach with the existing ones, namely dynamical density functional theory, classical Ginzburg-Landau theory, and also with quantum field theories.

References: [1] D. S. Dean, J. Phys. A: Math. Gen., 29, L613 (1996). [2] D. S. Dean and M. Krüger, J. Chem. Phys. 146, 134507 (2017). [3] M. Krüger et al, J. Chem. Phys. 148, 084503 (2018).

DY 30.7 Wed 12:00 H6

Coarsening dynamics of the long-range Ising model — Henrik Christiansen, Suman Majumder, and •Wolfhard Janke — Institut für Theoretische Physik, Universität Leipzig, Postfach 100 920, 04009 Leipzig, Germany

We report Monte Carlo computer simulations of the nonequilibrium coarsening dynamics of the two-dimensional long-range Ising model. Employing an efficient update scheme, our simulations perform $\sim 10^3$ times faster than the standard approach. We carefully examine previous approaches introducing a cut-off in the long-range potential in order to reduce the computational effort. Special emphasis is put on

a careful analysis of finite-size effects. This enables us to establish agreement with a theoretical prediction for the time dependence of the domain growth, in contrast to previous numerical studies. Our method can easily be generalized to applications in other systems.

[1] H. Christiansen, S. Majumder, and W. Janke, preprint arXiv:1808.10426.

DY 30.8 Wed 12:15 H6

Nonequilibrium monolayer of hard rods: Transient phase transition kinetics and phase boundaries — •Miriam Klopotek and Martin Oettel — Institute for Applied Physics, University of Tübingen, Germany

We perform kinetic Monte Carlo simulations of an idealized lattice model of hard rods with 'sticky' attractions, confined to a monolayer, diffusing under nonequilibrium conditions [1]. The simulations unveil rich (transient) phase transition kinetics including liquid-liquid phase separation, two-step cluster growth, and transient percolation, often enhanced by the strong driving forces: deposition, desorption or heating. In fact, these 'push' the system through its phase diagram, allowing us to map out the boundaries via 'kinks' or 'jumps' in both dynamical and structural observables: it matches the topology of the phase diagram predicted by density functional theory [2]. Our findings may be of direct relevance for experiments of thin film growth with organic molecules such as Pentacene in the first few layers [3], as well as simulations thereof [4,5].

[1] Klopotek *et al.*, *J. Chem. Phys* **146**, 084903 (2017).
[2] Mortazavifar and Oettel, *Phys. Rev. E* **96**, 032608 (2017).
[3] Zhang *et al.*, *Phys. Status Solidi RRL* **12**, 1800230 (2018).
[4] Roscioni *et al.*, *J Phys. Chem. Lett.* **9**, 6900 (2018).
[5] Clancy, *Chem. Mater.* **23**, 522 (2011).

DY 30.9 Wed 12:30 H6

Response of active Brownian particles to shear flow — •Kiryl Asheichyk[1,2], Alexandre Solon[3], Christian Rohwer[1,2], and Matthias Krüger[4] — [1]4th Institute for Theoretical Physics, University of Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Max Planck Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany — [3]Sorbonne University, CNRS, LPTMC, F-75005 Paris, France — [4]Institute for Theoretical Physics, University of Göttingen, 37073 Göttingen, Germany

We study the linear response of interacting active Brownian particles to simple shear flow. Using the path integral approach, we derive the linear response of any state observable after starting shear in terms of correlation functions evaluated for the unperturbed system. For systems and observables which are symmetric under exchange of x and y coordinates, the response formula can be drastically simplified to a form containing only state variables in the corresponding correlation functions (compared to the generic formula containing also time derivatives). The shear couples to the particles by both translational and rotational advection. In the mentioned case of symmetry, we also show that only translational advection is relevant in the linear regime. We apply the obtained formulas analytically and numerically to specific model setups. In particular, we investigate the morphology of a cluster of confined active interacting particles in shear flow, where we show that the activity increases the response.