DY 9: Statistical Physics far from Thermal Equilibrium

Time: Monday 10:00–13:30 Location: BH-N 334

DY 9.1 Mon 10:00 BH-N 334

An electronic Maxwell demon in the coherent strong-coupling regime — •Gernot Schaller[1], Javier Cerrillo[1], Geort Engelhardt[1], and Philipp Strasberg[2] — [1]Institut für Theoretische Physik, TU Berlin — [2]Physics and Materials Science Research Unit, Uni Luxembourg

We consider feedback control on a single electron transistor. Monitoring the occupation of the dot, conditional control operations can be interpreted as the action of a Maxwell demon. This can generate a current against a potential bias, producing electric power from information. While this is well-explored in the weak-coupling limit and has recently been implemented [1], we can address the strong-coupling regime with a collective mapping [2]. A continuous projective measurement of the central dot would lead to a complete suppression of electronic transport due to the quantum Zeno effect [3]. However, a microscopic model implements a weak measurement, which allows for closure of the control loop without inducing complete transport blockade [4]. In the weak-coupling regime, the energy flows associated with the feedback loop are negligible, and the information gained in the measurement bounds the generated electric power. In contrast, in the strong coupling limit, the protocol requires more energy than electric power produced, removing Maxwell's demon.

[1] K. Chida *et al.*, Nat. Comm. **8**, 15310 (2017).
[2] P. Strasberg *et al.*, arXiv:1711.08914.
[3] G. Engelhardt and G. Schaller, arXiv:1710.06306.
[4] G. Schaller *et al.*, arXiv:1711.00706.

DY 9.2 Mon 10:15 BH-N 334

Qubit absorption refrigerator at strong coupling — Anqui Mu[1], Bijay Kumar Agarwalla[2], •Gernot Schaller[3], and Dvira Segal[1] — [1]Dept. of Chemistry, University of Toronto — [2]Dept. of Physics, Indian Inst. of Science Education and Research — [3]Institut f. Theoretische Physik, TU Berlin

We demonstrate that a quantum absorption refrigerator can be realized from the smallest quantum system, a qubit, by coupling it in a non-additive (strong) manner to three heat baths. This function is un-attainable for the qubit model under the weak system-bath coupling limit, when the dissipation is additive. We obtain then closed expressions for the cooling window and refrigeration efficiency, as well as bounds for the maximal cooling efficiency and the efficiency at maximal power. Our results agree with macroscopic designs and with three-level models for quantum absorption refrigerators, which are based on the weak system-bath coupling assumption. Our work demonstrates that strongly-coupled quantum machines can exhibit function that is un-attainable under the weak system-bath coupling assumption.

[1] A. Mu *et al.*, NJP in press, arXiv:1709.02835.

DY 9.3 Mon 10:30 BH-N 334

Energy efficient quantum machines — •Obinna Abah[1] and Eric Lutz[2] — [1]Centre for Theoretical Atomic, Molecular and Optical Physics, Queen's University Belfast, United Kingdom. — [2]Department of Physics, University of Erlangen-Nuremberg, Germany.

We investigate the performance of a quantum thermal machine operating in finite time based on shortcut-to-adiabaticity techniques. We compute efficiency and power for a paradigmatic harmonic quantum Otto engine by taking the energetic cost of the shortcut driving explicitly into account. We demonstrate that shortcut-to-adiabaticity machines outperform conventional ones for fast cycles. We further derive generic upper bounds on both quantities, valid for any heat engine cycle, using the notion of quantum speed limit for driven systems. We establish that these quantum bounds are tighter than those stemming from the second law of thermodynamics.

Reference: Obinna Abah and Eric Lutz, EPL 118, 40005 (2017).

DY 9.4 Mon 10:45 BH-N 334

Diverging, but negligible power at Carnot efficiency: theory and experiment — •Viktor Holubec[1,2] and Artem Ryabov[2] — [1]Institut für Theoretische Physik, Universität Leipzig, Brüderstraße 15, 04103 Leipzig, Germany — [2]Charles University, Faculty of Mathematics and Physics, Department of Macromolecular Physics, V Holešovičkách 2, 18000 Praha, Czech Republic

We discuss the possibility of reaching the Carnot efficiency by heat engines (HEs) out of quasi-static conditions at nonzero power output. We focus on several models widely used to describe the performance of actual HEs. These models comprise quantum thermoelectric devices, linear irreversible HEs, minimally nonlinear irreversible HEs, HEs working in the regime of low dissipation, over-damped stochastic HEs and an under-damped stochastic HE. Although some of these HEs can reach the Carnot efficiency at nonzero and even diverging power, the magnitude of this power is always negligible compared to the maximum power attainable in these systems. We provide conditions for attaining the Carnot efficiency in the individual models and explain practical aspects connected with reaching the Carnot efficiency at large power output. Furthermore, we show how our findings can be tested in practice using a standard Brownian HE realizable with available micromanipulation techniques.

DY 9.5 Mon 11:00 BH-N 334

Quantum heat engines and laser cooling: A study beyond the weak coupling and Markovian approximations — •Sebastian Restrepo[1], Javier Cerrillo[1], Philipp Strasberg[2], and Gernot Schaller[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Complex Systems and Statistical Mechanics, University of Luxembourg, Luxembourg

We study a periodically driven thermal machine beyond the weak coupling and Markovian approximations by combining a collective coordinate mapping with Floquet theory and full counting statistics. We identify a collective degree of freedom in the reservoir that is included as part of an enlarged supersystem to take strong coupling and non-Markovian effects into account. The periodicity of our extended model is exploited using Floquet theory to obtain a master equation with full counting statistics methods permitting a thermodynamic analysis. The formalism is applied to a thermal machine consisting of a driven two-level system coupled to two reservoirs at different temperatures with one of the couplings considered time-dependent. In the weak-coupling regime, the setup can switch between the operational modes of a heat engine or a refrigerator directly. As the coupling is increased, we identify four different operation regimes and see the eventual disappearance of the refrigerator. We observe that the efficiency and coefficient of performance decrease for stronger couplings. Taking the limit of a single reservoir, our model is able to replicate the setup of state preparation in laser cooling of trapped ions.

DY 9.6 Mon 11:15 BH-N 334

Singularity in large deviations of work in quantum quenches — •Pietro Rotondo, Jiri Minar, Igor Lesanovsky, Juan P. Garrahan, and Matteo Marcuzzi — University of Nottingham, School of Physics and Astronomy, University Park NG7 2RD

We investigate the large deviations of the work performed in a quantum quench across two different phases separated by a quantum critical point. We analyse the Dicke model as a paradigmatic example, and employ an approximate description, valid in each phase in the thermodynamic limit, which reduces it to a set of two harmonic oscillators. We identify large deviations forms for the corresponding Loschmidt amplitude and its conjugate functional, the distribution of the work. We then compare these findings with the predictions of a recently-proposed classification scheme put forward in [Phys. Rev. Lett. 109, 250602 (2012)]. For certain values of the parameters, we highlight a regime going beyond the ones listed in this classification. In these cases, the rate function exhibits a non-analytical point, a strong indication of the presence of an out-of-equilibrium phase transition in the functional describing the rare fluctuations of the work.

DY 9.7 Mon 11:30 BH-N 334

Correlational latent heat by nonlocal quantum kinetic theory — •Klaus Morawetz — Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil — Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany

The nonlocal kinetic equation unifies the achievements of the transport in dense quantum gases with the Landau theory of quasiclassical transport in Fermi systems. Large cancellations in the off-shell motion appear which are hidden usually in non-Markovian behaviors [1]. The remaining corrections are expressed in terms of shifts in space and time that characterize the non-locality of the scattering process [2]. In this way quantum transport is possible to recast into a quasi-classical picture [3]. The balance equations for the density, momentum, energy and entropy include besides quasiparticle also the correlated two-particle contributions beyond the Landau theory [4]. The medium effects on binary collisions are shown to mediate the latent heat, i.e., an energy conversion between correlation and thermal energy. For Maxwellian particles a sign change of the latent heat is reported at a universal ratio of scattering length to the thermal De Broglie wavelength. This is interpreted as a change from correlational heating to cooling. [1] Ann. Phys. 294 (2001) 135, [2] Phys. Rev. C 59 (1999) 3052, [3] "'Interacting Systems far from Equilibrium -Quantum Kinetic Theory"', Oxford University Press, (2017), ISBN 9780198797241, [4] Phys. Rev. E 96 (2017) 032106

15 min. break

DY 9.8 Mon 12:00 BH-N 334

Thermodynamic signatures of shear-induced transitions in confined colloidal suspensions in shear flow — •Sascha Gerloff and Sabine H. L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

Colloidal suspensions under the combined influence of shear flow and strong spatial confinement display a rich non-equilibrium behavior [1]. One intriguing question is how these dynamical transitions are reflected by macroscopic quantities, such as the shear stress and thermodynamic functions. Here, we perform overdamped *Brownian* dynamic (BD) simulations of charged colloids under shear flow confined to a narrow slitpore. In equilibrium, the colloids organize in crystalline layers, whose in-plane structure depends on the slitpore width [2]. Applying shear flow introduces new types of structural transitions driven by the collective motion of the colloids [1]. We investigate the work- and heat rate, as well as the entropy production related to different steady states. These quantities are calculated from particle trajectories in the spirit of stochastic thermodynamics [3]. We find that transitions between different steady states are reflected in these thermodynamic quantities. In particular, the work- and heat rates are closely related to the shear stress, which characterizes the rheological response of the system.

[1] S. Gerloff and S. H. L. Klapp, *Phys. Rev. E* **94**, 062605 (2016).
[2] A. Fortini and M. Dijkstra, *J. Phys. Condens. Matter* **18**, L371 (2006).
[3] T. Speck and U. Seifert, *Phys. Rev. E* **79**, 178302 (2009).

DY 9.9 Mon 12:15 BH-N 334

Oscillating Modes of Driven Colloids in Overdamped Systems — •Johannes Berner[1], Boris Müller[2,3], Juan Ruben Gomez-Solano[1], Matthias Krüger[2,3], and Clemens Bechinger[1] — [1]Physics Department, University of Konstanz, 78457 Konstanz, Germany — [2]4th Institute for Theoretical Physics, University of Stuttgart, 70569 Stuttgart, Germany — [3]Max Planck Institute for Intelligent Systems, Heisenbergstrasse 3, 70569 Stuttgart, Germany

Microscopic particles suspended in liquids are the prime example of an overdamped system because viscous forces dominate over inertial effects. Apart from their use as model systems, they receive considerable attention as sensitive probes from which forces on molecular scales can be inferred. The interpretation of such experiments rests on the assumption, that, even if the particles are driven, the liquid remains in equilibrium, and all modes are overdamped. Here, we experimentally demonstrate that this is no longer valid when a particle is forced through a viscoelastic fluid. Even at small driving velocities where Stokes law remains valid, we observe particle oscillations with periods up to several tens of seconds. We attribute these to non-equilibrium fluctuations of the fluid, which are excited by the particle's motion. The observed oscillatory dynamics is in quantitative agreement with an overdamped Langevin equation with negative friction-memory term and which is equivalent to the motion of a stochastically driven underdamped oscillator. This fundamentally new oscillatory mode has considerable implications on how molecular forces are determined by colloidal probe particles under natural viscoelastic conditions.

DY 9.10 Mon 12:30 BH-N 334

On the generalized generalized Langevin equation : a non-stationary approach of the Mori-Zwanzig formalism — •Hugues Meyer[1], Thomas Voigtmann[2], and Tanja Schilling[3] — [1]Université du Luxembourg, Esch-sur-Alzette, Luxemburg — [2]Albert-Ludwigs-Universität, Freiburg-im-Breisgau, Germany — [3]DLR, Köln, Germany

As a researcher in statistical physics, one may often be interested in reducing the complexity of a many-particle system to the study of a set of relevant observables (for instance, the system could be a polymer melt and the aim could be to develop a rheological model). This procedure is called coarse-graining as soon as the timescale of these variables is much larger than the microscopic timescale. A systematic way to derive an equation of motion for these observables from the microscopic dynamics is known for some time as the Mori-Zwanzig formalism and leads to the generalized Langevin equation. In contrast, if the dynamics is not stationary, it is not a priori clear which form the equation of motion for an averaged observable has. We adapt this formalism to derive the equation of motion for a non-equilibrium trajectory-averaged observable as well as for its non-stationary autocorrelation function. We also derive a fluctuation-dissipation-like relation which relates the memory kernel and the autocorrelation function of the fluctuating force. In addition, we show how to relate the Taylor expansion of the memory kernel to experimental data, thus allowing to construct the equation of motion from direct measurements. We finally illustrate this method on various simple examples.

DY 9.11 Mon 12:45 BH-N 334

Investigating the Reaction Dynamics for a Thermally Coupled System with a Rank-1 Saddle Potential — •Robin Bardakcioglu, Philippe Schraft, Johannes Reiff, Martin Tschöpe, Matthias Feldmaier, Jörg Main, and Günter Wunner — 1. Institut für Theoretische Physik, Universität Stuttgart, Germany

Transition State Theory provides an atomistic approach to the calculation and prediction of chemical reaction rates. By analyzing classical equations of motion for a molecular system, one can determine the reactant and product regions in phase space. With the use of an invariant manifold approach, we can find recrossing-free dividing surfaces between these regions, which allow us to determine the reaction rate for an open, time-dependently driven system. We use these methods to investigate the reaction dynamics of a system subject to Langevin dynamics, i.e. thermal noise.

DY 9.12 Mon 13:00 BH-N 334

Localized Deposition - Controlling cluster growth far from thermal equilibrium — •Thomas Martynec, Benedikt Hartung, and Sabine H.L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Berlin, Germany

Thin-film growth by means of molecular beam epitaxy (MBE) is a typical example of non-equilibrium growth and a powerful method to produce devices for various technological applications [1-2]. Initially, particles are deposited at constant rate F on an empty lattice where these monomers freely diffuse until they meet other free particles on the lattice to form clusters. Nucleation events are randomly distributed on the lattice and one can only control the number of nucleation events (by varying temperature T and adsorption rate F) but not the location. This can be circumvented by using a stencil (or shadow) mask of linear size l [3-4]. Varying the size l, the particle flux F and the temperature T allows to spatially control nucleation events and the shape of clusters. We perform kinetic Monte-Carlo (KMC) simulations with spatially localized flux and identify three different growth modes that also emerge in experiments [4-5].

[1] S. Liu et al., npj 2D Materials and Applications **1**, 30 (2017)
[2] Parkes et al., Sci Rep. **3**, 2220 (2013)
[3] H. Yun et al., Sci Rep. **5**, 10220 (2015)
[4] P. Fesenko et al., Cryst. Growth Des. **16**, 4694 (2016)
[5] T. Martynec, B. Hartung, and S. H. L. Klapp, in preparation

DY 9.13 Mon 13:15 BH-N 334

Effective thermodynamics for a marginal observer — •Matteo Polettini and Massimiliano Esposito — Physics and Materials Science Research Unit, University of Luxembourg, Campus Limpertsberg, 162a avenue de la Faiencerie, L-1511 Luxembourg (Luxembourg)

Thermodynamics often presumes that the observer has complete information about the system she or he deals with: no parasitic current, exact evaluation of the forces needed to drive the system out of equilibrium. However, most often the observer only measures marginal information. How is she or he to make consistent thermodynamic claims? Disregarding sources of dissipation might lead to bold claims, such as the possibility of perpetuum mobile. We show that it is nevertheless possible to produce an effective description that does not dispense with the fundamentals of thermodynamics: the 2nd Law, the Fluctuation-Dissipation paradigm, and the more recent and encompassing Fluctuation Theorem.