DY 8: Statistical Physics far from Thermal Equilibrium

Time: Monday 15:00–19:15 Location: ZEU 118

DY 8.1 Mon 15:00 ZEU 118

Enhanced nonequilibrium fluctuations of particles driven through a viscoelastic bath — •Johannes Berner[1], Juan Ruben Gomez-Solano[1], and Clemens Bechinger[1,2] — [1]2. Phykalisches Institut, Universität Stuttgart, Germany — [2]MPI for Intelligent Systems, Stuttgart, Germany

Viscoelastic fluids are of great importance in biological systems and in medical and industrial applications. Their flow properties have been extensively studied by bulk rheology [1] and more recently by microrheology [2] using embedded colloidal probes. For instance in passive microrheology the fluctuation-dissipation theorem is used to determine such properties by measuring the thermal fluctuations of the particle position [3]. This is only valid provided that the fluid and the particle are in thermal equilibrium. However this assumption is not trivially satisfied, if the microstructure of the fluid is driven far from equilibrium, e.g. by inducing a local deformation by means of the particle [4, 5]. In this work, we investigate the fluctuations of a colloidal particle driven by optical tweezers at constant velocity through a viscoelastic medium. Unlike in a Newtonian fluid, we observe an enhancement of those fluctuations by driving the fluid out of equilibrium.

[1] Larson R G 1999 The Structure and Rheology of Complex Fluids (New York: Oxford University Press), [2] Squires T. M. and Mason T. G., Annu. Rev. Fluid Mech., 42 (2010) 413, [3] Mason T. G. and Weitz D. A., Phys. Rev. Lett., 74 (1995) 1250, [4] Gomez-Solano J. R. and Bechinger C., EPL, 108 (2014) 54008, [5] Gomez-Solano J. R. and Bechinger C., New J. Physics, 17 (2015) 103032

DY 8.2 Mon 15:15 ZEU 118

Nonequilibrium thermodynamics in the strong coupling and non-Markovian regime based on a reaction coordinate mapping — •Philipp Strasberg[1], Gernot Schaller[1], Neill Lambert[2], and Tobias Brandes[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, Germany — [2]CEMS, RIKEN, Saitama, 351-0198, Japan

We propose a method to study the thermodynamic behaviour of small systems beyond the weak coupling and Markovian approximation, which is different in spirit from conventional approaches. The idea is to redefine the system and environment such that the effective, redefined system is again coupled weakly to Markovian residual baths and thus, allows to derive a consistent thermodynamic framework for this new system-environment partition. To achieve this goal we make use of the reaction coordinate mapping, which is a general method in the sense that it can be applied to an arbitrary (quantum or classical and even time-dependent) system coupled linearly to an arbitrary number of harmonic oscillator reservoirs. We demonstrate the power of this concept by showing that non-Markovian effects can significantly enhance the steady state efficiency of a three-level-maser heat engine, even in the regime of weak system-bath coupling.

Reference: New. J. Phys. 18, 073007

DY 8.3 Mon 15:30 ZEU 118

Bridging the gap between atomistic and macroscopic models of homogeneous nucleation — •Bingqing Cheng[1], Gareth Tribello[2], and Michele Ceriotti[1] — [1]EPFL, Lausanne, Switzerland — [2]Queen's University Belfast, Belfast, UK

Nucleation has many implications in science and technology, including metal casting, the assembly of microtubules in cells, and the formation of water droplets in the atmosphere. Because the experimental investigation of dynamical nucleation processes is very difficult, much attention has been paid to atomistic simulation efforts in the last two decades.

However, atomistic simulation studies of nucleation face two major challenges. Firstly, the free energy barrier separating the metastable phase and the stable phase can be very high, making nucleation times much larger than the time scales accessible to molecular dynamics simulations. Secondly, it is highly non-trivial to develop a predictive macroscopic model of nucleation using the microscopic quantities directly obtained from atomistic simulations.

In this talk, I aim to address the aforementioned difficulties. I will first briefly introduce state-of-the-art enhanced sampling methods for atomistic simulations, and their applications to studying homogeneous nucleation. I will then discuss our latest thermodynamic model that links macroscopic theories and atomic-scale simulations and thus provide a simple and elegant framework to verify and extend classical nucleation theory.

DY 8.4 Mon 15:45 ZEU 118

Nonequilibrium thermodynamics by nonlocal quantum kinetic theory — •Klaus Morawetz[1,2,3] and Pavel Lipavsky[4] — [1]Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics (IIP) Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil — [3]Max-Planck-Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [4]Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, 12116 Prague 2, Czech Republic

The balances for thermodynamic quantities are derived from the nonlocal kinetic quantum kinetic equation. It turns out that the nonlocal collision scenario leads to molecular contributions to the observables and currents. The corresponding observable is multiplied with the rate to form a molecule and the delay time which can be considered as collision duration. Explicit expressions of these molecular contributions are given in terms of the scattering phase shifts. The two-particle form of the entropy is derived. This extends the Landau quasiparticle picture by two-particle molecular contributions. While for energy and momentum there is a continuous exchange of correlation into kinetic parts condensing into the rate of correlated variables. For the entropy an explicit gain remains and Boltzmann's H-theorem is proved including the molecular parts of entropy. The consistency of the theory is shown by obtaining the same expressions from the functional between Wigner and quasiparticle distribution within the extended quasiparticle picture.

DY 8.5 Mon 16:00 ZEU 118

Bethe-ansatz solution for ASEP with reflecting boundaries and its application to polymer dynamics — •Wenwen Huang, YenTing Lin, Daniela Frömberg, Frank Jülicher, and Vasily Zaburdaev — Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

In this contribution, we show that the exact solution of Asymmetric Simple Exclusion Process (ASEP) with reflecting boundaries can be found using a generalised Bethe-ansatz method. The exact partition function is derived and thus the stationary density profile can be solved exactly. Moreover, we calculate the eigenvalues and eigenfunctions of the system analytically and discuss the slowest relaxation time. In addition, we show how to map the ASEP setting to the dynamics of a pinned polymer loop system. By using this mapping, we can get insights into the equilibrium statistics and dynamics of the polymer system. Furthermore, we show how the generalised Bethe-ansatz method can be applied to the continuous single-file diffusion with reflecting boundaries.

DY 8.6 Mon 16:15 ZEU 118

Quantum thermodynamics with local control — •Rodrigo Gallego[1], Jaqueline Lekscha[1,2,3], Henrik Wilming[1], and Jens Eisert[1] — [1]Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany — [2]Potsdam Institute for Climate Impact Research, 14473 Potsdam, Germany — [3]Department of PHysics, Humboldt-Universität zu Berlin, 12489 Berlin, Germnay

We investigate the limitations that emerge in thermodynamic tasks as a result of having local control only over the components of a thermal machine. These limitations are particularly relevant for devices composed of interacting many-body systems. Specifically, we study protocols of work extraction that employ a many-body system as a working medium whose evolution can be driven by tuning the on-site Hamiltonian terms. This provides a restricted set of thermodynamic operations, giving rise to novel bounds for the performance of engines. Our findings show that those limitations in control render it in general impossible to reach Carnot efficiency; in its extreme ramification it can even forbid to reach a finite efficiency or finite work per particle. We focus on the 1D Ising model in the thermodynamic limit as a case study. We show that in the limit of strong interactions the ferromagnetic case becomes useless for work extraction, while the anti-ferromagnetic improves its performance with the strength of the couplings, reaching Carnot in the limit of arbitrary strong interactions. Our results pro-

vide a promising connection between the study of quantum control and thermodynamics and introduce a more realistic set of physical operations well suited to capture current experimental scenarios.

DY 8.7 Mon 16:30 ZEU 118

Driven open quantum systems and Floquet stroboscopic dynamics — •Sebastian Restrepo[1], Javier Cerrillo[1], Victor M. Bastidas[2], Dimitri Angelakis[2], and Tobias Brandes[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Centre for Quantum Technologies, National University of Singapore, 3 Science Drive 2, Singapore

We provide an analytic solution to the problem of driven open quantum systems at the high-frequency limit that goes beyond the weak coupling and Markovian assumptions. It may be applied for the study of driven-dissipative many-body systems, since it solely relies on discrete symmetries of the system-bath Hamiltonian and provides the time evolution operator of the full Hilbert space, including bath degrees of freedom. This allows us to see both the effects of the driving on the coherent part of the dynamics and also on the environment (dissipation).

We propose an interpretation of the solution for the driven open system in terms of the stroboscopic evolution of a continuous family of observables under the influence of an effective static Hamiltonian. The interpretation constitutes a flexible simulation procedure of non-trivial static Hamiltonians. We instantiate the result with the study of the spin-boson model with time-dependent tunneling amplitude and provide observations of simulated polaron dynamics in the strong coupling limit.

15 min. break

DY 8.8 Mon 17:00 ZEU 118

Driven quantum baths — •Joscha Reichert[1,2], Peter Nalbach[3], Hermann Grabert[4,5], and Michael Thorwart[1,2] — [1]I. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, 20355 Hamburg, Germany — [2]The Hamburg Centre for Ultrafast Imaging, Luruper Chaussee 149, 22761 Hamburg, Germany — [3]Westfälische Hochschule, Münsterstraße 265, 46397 Bocholt, Germany — [4]Freiburg Institute for Advanced Studies (FRIAS), Universität Freiburg, Albertstr. 19, 79104 Freiburg, Germany — [5]Physikalisches Institut, Universität Freiburg, Hermann-Herder-Straße 3, 79104 Freiburg, Germany

The established theoretical framework of quantum dissipation usually neglects the interaction between a probing pulse and the surrounding environment of a central-quantum system to preserve equilibrium conditions. The introduction of a dipolar coupling to the environmental modes gives rise to an additional force-component on the system in question which can be quantified using a simple dielectric solvation model. An investigation for a THz-probed polarizable molecule in water and a quantum-dot metal-nanoparticle setup leads to enhancement and profound changes in the linear response of both systems [1]. A more detailed investigation of the spin-boson model within a master-equation framework and pulse-shaped bath-driving reveals the additional force to capture the non-equilibrium memory effects of the bath and depends on its underlying spectral characteristics [2].

[1] Phys. Chem. Lett. 7, 2015 (2016)
[2] Phys. Rev. A 94, 032127 (2016)

DY 8.9 Mon 17:15 ZEU 118

Jarzynski equality beyond thermal Gibbs states — •Daniel Schmidtke and Jochen Gemmer — Fachbereich Physik, Universität Osnabrück, Germany

The Jarzynski equality allows to derive equilibrium thermodynamical quantities just from irreversible (non-equilibrium) trajectories. It holds in both, the classical and the quantum context. Though settings and approaches indeed differ greatly, they all have in common that the initial state is some thermal Gibbs state. Up to now, no conclusive theory when considering other initial states is presented. Therefore, we numerically investigate work distributions in driven isolated systems, starting off from single energy eigenstates of the initial Hamiltonian. A finite size scaling might allow for statements on whether the Jarzynski equality must require Gibbs states, or other initial states at least will fulfill this relation to good accuracy. Moreover, we point out the close connection between fulfilling the Jarzynski equality and eigenstate thermalization hypothesis.

DY 8.10 Mon 17:30 ZEU 118

Manipulating decoherence and relexation by adding non-commuting noise — •Timo Palm[1,2] and Peter Nalbach[1] — [1]Westfälische Hocheschule ,Münsterstr. 265 , 46397 Bocholt — [2]I. Institut für Theoretische Physik Universität Hamburg Jungiusstraße 9 20355 Hamburg

In recent years the role of coherence in quantum systems has been a field of increasing interests, with applications reaching from quantum dots and quantum computers to solar cell efficiency and the possible use of such mechanisms in artificial light-harvesting complexes. Interaction of such quantum system with environments typically destroys coherence and yields relaxation, with larger coupling strengths to the environment resulting in faster relaxation/decoherence. We show that the relaxation rates can significantly be reduced by adding environmental fluctuations, which couple via non-commuting system bath operators. As a toy model the two level system is studied, its dynamics is simulated via an extended version of the quasi adiabatic path integral and a perturbative theory (RESPET).

DY 8.11 Mon 17:45 ZEU 118

Universality of entropy production in driven diffusions — •Simone Pigolotti, Izaak Neri, Édgar Roldán, and Frank Jülicher — Max-Planck Institute for the Physics of Complex Systems, Dresden, Germany

We study non-equilibrium properties of driven colloidal systems, ranging from simple one-dimensional periodic potentials to two-dimensional incompressible flows. We will show that some statistical properties of the entropy production, such as the distribution of local infima, are universal at steady state. We develop a general theory to account for these findings. We conclude with an example of a system maintained out of steady-state by a time-dependent driving which, surprisingly, shares the same universal properties.

DY 8.12 Mon 18:00 ZEU 118

Reducing the roughness in non-equilibrium surface growth by controlled temperature modulations — •Thomas Martynec and Sabine H.L. Klapp — Institut für Theoretische Physik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

The non-equilibrium crystal growth often leads to undesired rough interfaces which negatively affect the quality of devices. By controlled temperature modulations during the non-equilibrium growth it is possible to overcome this problem and obtain smoother structures. The idea is based on the concept of two mobilities [1] which is realized by using different temperatures T during the growth such that the nucleation length associated with second layer nucleation is changed. Using a low temperature T in the early stage of growth and increasing it during the growth leads to small islands and reduces the rate of second layer nucleation. The goal is to find optimal T-modulations by means of kinetic Monte-Carlo simulations such that coalescence of clusters sets in before it comes to nucleation in the layer above and the structure growths in a layer-by-layer fashion.

[1] G. Rosenfeld, B. Poelsema, G. Comsa, J. Cryst. Growth 151, 230-233 (1995)
[2] R. Kunkel, B. Poelsema, L. K. Verheij, G. Comsa, Phys. Rev. Lett. 65, 733 (1990)
[3] P. Šmilauer, M. R. Wilby, D. D. Vvedensky, Phys. Rev. B 47, 4119(R) (1993)
[4] S. Kowarik et al., unpublished.

DY 8.13 Mon 18:15 ZEU 118

The third law for finite non-equilibrium resources — •Henrik Wilming and Rodrigo Gallego — Dahlem Center for Complex Quantum Systems, Freie Universität Berlin, 14195 Berlin, Germany

The third law in the form of the unattainability principle states that exact ground-state cooling requires infinite resources. Here we investigate the amount of resources needed for approximate cooling. We consider as resource any system out of equilibrium, allowing for resources beyond the i.i.d. assumption and including the input of work as a particular case. We establish sufficient conditions for cooling in full generality and show that for a vast class of non-equilibrium resources sufficient and necessary conditions for low-temperature cooling can be expressed in terms of a single function. This function plays a similar role for the third law to the one of the free energy for the second law. From a technical point of view we provide new results about concavity/convexity of certain Renyi-divergences, which might be of independent interest.

DY 8.14 Mon 18:30 ZEU 118

Fluctuation-dissipation relations far from equilibrium — •Bernhard Altaner, Matteo Polettini, and Massimiliano Esposito — Complex Systems and Statistical Mechanics, Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg

Near equilibrium, where all currents of a system vanish on average, the fluctuation-dissipation relation (FDR) connects a current's spontaneous fluctuations with its response to perturbations of the conjugate thermodynamic force. Out of equilibrium, fluctuation-response relations generally involve additional nondissipative contributions. Here, in the framework of stochastic thermodynamics, we show that an equilibrium-like FDR holds for internally equilibrated currents, if the perturbing conjugate force only affects the microscopic transitions that contribute to the current. We discuss the physical requirements for the validity of our result and apply it to nano-sized electronic devices.

Reference: Phys. Rev. Lett. 117, 180601

DY 8.15 Mon 18:45 ZEU 118

Solvent Coarsening around a Colloid upon Cooling — •Sutapa Roy[1], S Dietrich[1], and Ania Maciolek[2] — [1]Max-Planck-Institut für Intelligente Systeme, Heisenbergstr. 3, 70569 Stuttgart, Germany and IV. Institut für Theoretische Physik, Universität Stuttgart, Pfaffenwaldring 57, 70569 Stuttgart, Germany — [2]Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, PL-01-224 Warsaw, Poland

We investigate temperature-gradient induced coarsening of a cooling binary solvent around a spherical colloidal particle, using numerical calculations and analytical theory. Our phenomenological model impersonates recent experiments in which, upon laser heating of a Janus colloid, the surrounding binary liquid mixture develops concentration gradient. Evidence of 'non-localized' coarsening is provided around a Janus colloid even if the colloid temperature is above the bulk demixing critical temperature of the solvent.

DY 8.16 Mon 19:00 ZEU 118

Depinning as a coagulation process — •Muhittin Mungan[1], Melih Iseri[1], and David Kaspar[2] — [1]Department of Physics,, Bogazici University, 34342 Istanbul, Turkey — [2]Division of Applied Mathematics, Brown University, Providence, RI 02912, USA

We consider a one-dimensional sandpile model which mimics an elastic string of particles driven through a strongly pinning periodic environment with phase disorder.

The evolution towards depinning occurs by the triggering of avalanches in regions of activity which are at first isolated but later grow and merge. For large system sizes the dynamically critical behavior is dominated by the coagulation of these active regions. The analysis and numerical simulations show that the evolution of the sizes of active regions is well-described by a Smoluchowski coagulation equation, allowing us to predict correlation lengths and avalanche sizes. Moreover, the coagulation process emerges as the macroscopic description of the evolution to depinning.

As our analysis shows, this connection is robust, i.e. it depends little on the details of the underlying microscopic model, providing an example for the emergence of universal features in disordered systems far from equilibrium.