DY 55: Poster: Noneq. Stat. Phys., Stat. Bio. Phys., Brownian

Time: Thursday 15:00–18:00 Location: Poster B2

DY 55.1 Thu 15:00 Poster B2

Coherent oscillations in periodically driven systems — •Lukas Oberreiter[1], Andre Cardoso Barato[2], and Udo Seifert[1] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany — [2]Department of Physics, University of Houston, Houston, Texas 77204, USA

Biochemical oscillations are prevalent in living organisms. Organisms count time with biochemical oscillators to properly time their functions. Since these oscillations rely on a stochastic process fluctuations in the period of oscillation lead to a finite precision. The latter is quantified by the number of coherent oscillations. A former study [1] revealed that the number of coherent oscillations of an autonomous system is bounded by the topology of the network of states and the thermodynamic force that drives the system out of equilibrium. Here, we extend the analysis to *periodically* driven systems. We construct a specific external protocol showing that the number of coherent oscillations is not necessarily bounded. Moreover, the trade-off between the number of coherent oscillations and its costs, the entropy production rate, is investigated.

[1] A. C. Barato and U. Seifert, Phys. Rev. E **95**, 062409 (2017)

DY 55.2 Thu 15:00 Poster B2

Coarse-grained toy model for ring polymer melts — •Stanard Mebwe Pachong[1], Jan Smrek[2], and Kurt Kremer[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]University of Vienna, Austria

Nonconcatenated and unknotted rings in melt subdiffuse on length scales several times larger than their gyration radius [1]. It has been hypothesised that ring threadings [2,3], although they might be quantitatively marginal [4]. On the other hand, the prolonged onset of diffusion can be observed also in a dense system with a small number of particles with a relatively deep correlation hole. Due to a finite-size effect, a significant rearrangement would be necessary for large particle displacements which results in longer sub-diffusion regime. As the simulated ring melts [1] were composed of only 200 rings and have deep correlation holes, the effect can be at play. In order to understand the cause of the subdiffusion of the rings melt, we attempt to falsify the threading hypothesis. We constructed a simple coarse-grained (soft-sphere) model of rings that (trivially) cannot thread, but can exhibit the correlation hole effect. We have not found a sign of subdiffusion. This goes in line with a recent observation that threading and diffusion relax on similar time scales[4].

References

[1] J. D. Halverson et al., J. Chem. Phys., 134,204905(2011) [2] Michieletto et al. ACS Macro Lett.,3,255-259(2014) [3] J. smrek and A. Y. Grosberg,ACS Macro Lett.5,750-754(2016) [4] J. Smrek, K. Kremer, A. Rosa ,unpublished(2018)

DY 55.3 Thu 15:00 Poster B2

Field Theoretic Thermodynamic Uncertainty Relation for the Kardar-Parisi-Zhang Equation — •Oliver Niggemann and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart

In this poster I will present a way to show the validity of the thermodynamic uncertainty relation in the setting of the one-dimensional Kardar-Parisi-Zhang (KPZ) equation with white in time, spatially colored Gaussian noise for weak coupling, i.e. $\partial_t h(x,t) = \nu\partial_x^2 h(x,t) + \lambda/2(\partial_x h(x,t))^2 + \eta(x,t)$ with $\langle\eta(x,t)\rangle = 0$ and $\langle\eta(x,t)\eta(x',t')\rangle = D(|x-x'|)\delta(t-t')$. Within Hilbert space theory of stochastic partial differential equations the height field $h(x,t)$ is regarded as a trajectory $t \mapsto h(x,t)$, $h(x,t) \in \mathcal{H}$. On a finite spatial interval $[0,L]$, $\mathcal{H} = \mathcal{L}_2(0,L)$ is a suitable choice, and the eigenfunctions of the differential operator $\mathcal{A} \equiv \nu\partial_x^2$ with periodic boundary conditions form an orthonormal base of $\mathcal{H}$. The height $h(x,t)$ and the noise $\eta(x,t)$ are expressed then by means of eigenfunction expansions. In this setting, the following thermodynamic uncertainty relation has been derived for the non-equilibrium steady state: $\Delta s_{\text{tot}}^{\text{stat}}\epsilon^2 > 2 + O(\lambda^2)$. Here $\Delta s_{\text{tot}}^{\text{stat}} \equiv \int_0^t dt' \left((\partial_x h(x,t'))^2, \hat{D}^{-1}(\partial_x h(x,t'))^2\right)_{\mathcal{L}_2}$ is the stationary state total entropy production, and $\epsilon^2 \equiv \langle\|h(x,t) - \langle h(x,t)\rangle\|_{\mathcal{L}_2}^2\rangle / \|\langle h(x,t)\rangle\|_{\mathcal{L}_2}^2$ is the squared variation coefficient of $h(x,t)$, evaluated for $t \gg 1$. $\hat{D}^{-1}$ is the inverse of the integral covariance operator with kernel $D(|x-x'|)$. The uncertainty relation holds for $D(x)$ describing a class of regular spatially colored noise, which, in a suitable limit, approximates white noise and for white noise itself, i.e. $D(x) = \delta(x)$.

DY 55.4 Thu 15:00 Poster B2

Hot Brownian Motion on Short Time Scales — •Xiaoya Su — Molecular Nanophotonics, Peter Debye Institute for Soft Matter Physics, University Leipzig, Linnéstraße 5, 04103, Leipzig

Hot Brownian motion describes the motion of a heated microsphere in a liquid. It is a fundamental issue for thermal non-equilibrium. A temperature field is created around the heated particle decaying with 1/r and a stationary temperature and viscosity field is moving with the particle through the liquid. The non-equilibrium dynamics of the particle now differs from the unheated particles and an effective temperature and viscosity is introduced to describe the system. Here we report on a study of the fluctuations of a heated particle in an optical trap with nanosecond and nanometer resolution. We calculated the mean squared displacement MSD and the autocorrelation function of velocity(VACF) of the heated particle and found evidence that the short time motion is influenced by the temperature increase.

DY 55.5 Thu 15:00 Poster B2

Characterizing non-equilibrium steady states via invariant manifolds — •Prakhar Godara, Jens Lucht, Marco Mazza, and Stephan Herminghaus — MPI für Dynamik und Selbstorganisation, Göttingen

It is still an unsolved question whether there is a general way to predict the steady state of a driven (non-equilibrium) system (a convection roll, a spiral wave, spatiotemporal chaos etc.) solely from its microscopic physics. The main obstacle is that detailed balance is breached in such systems. However, by describing the system not in state space, but instead in the space of all possible closed cycles in that space, detailed balance reappears. We demonstrate for the two-dimensional Fokker-Planck equation that the transition rates in this 'cycle space' can be obtained from simple integrals of the drift field and the diffusion field, yielding a general potential in cycle space. The occupation probabilities of the non-equilibrium steady states, which correspond to the invariant manifolds of the drift field, are then given by a Boltzmann factor containing this potential. We corroborate our findings numerically.

DY 55.6 Thu 15:00 Poster B2

Large deviations for a driven underdamped particle in a periodic potential — •Lukas P. Fischer and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, Germany

Large deviation theory is a versatile tool that proved useful for establishing connections between current fluctuations and thermodynamic steady state properties, e.g. the thermodynamic uncertainty relation [1]. Previous studies, however, were limited to systems which are diffusive in all variables, i.e. overdamped Brownian motion or Markov jump processes. In a previous study we extended the work to underdamped Brownian motion of a single, driven particle in a periodic potential and derived an expression for the large deviation functional of the empirical phase space density [2]. This functional replaces the level 2.5 functional used for overdamped dynamics. Although bounds can be derived from the underdamped level 2 functional in general, a straightforward proof of the thermodynamic uncertainty relation for underdamped dynamics is not possible. In this contribution we revisit the underdamped large deviation function for a driven particle in a periodic potential with focus on the thermodynamic uncertainty relation. We present some ansatzes for thermodynamic bounds and discuss the problems arising from them. Furthermore we outline difficulties which have to be faced following other techniques.

[1] A.C. Barato, U. Seifert, Phys. Rev. Lett. **114**, 158101 (2015)
[2] L.P. Fischer, P. Pietzonka, U. Seifert, Phys. Rev. E **97**, 022143, (2018)

DY 55.7 Thu 15:00 Poster B2

Dynamic ordering of driven spherocylinders in a non-equilibrium suspension of small colloidal spheres — •Anton Lüders, Ullrich Siems, and Peter Nielaba — Department of Physics, University of Konstanz, 78457 Konstanz, Germany

The ordering effects of driven spherocylinder-shaped rods in a colloidal suspension of small spheres confined to a two-dimensional channel geometry are observed via Brownian Dynamics simulations without hydrodynamics. To describe the ordering, an order parameter and an expression for a potential of mean force of an equivalent equilibrium system are defined and analyzed. By varying the application point of the external force along the rods and thus the resulting lever, a transition from a preferred orientation parallel to the direction of the force to a preferred orientation perpendicular to the direction of the force was observed. It is shown that this effect can only be found, if the spheres and multiple rods are present. Furthermore, a dependency of the order parameter on the absolute value of the force was discovered. The analysis of the potential of mean force further indicates a transition between two different phases of mean orientation. The observation of the flow equilibrium mean velocity in channel direction led to a s-shaped progression regarding the lever dependency, also marking a transition between two states linked to the mean orientation of the rods. By means of a finite size analysis it was possible to show that the transition between the two orientation states is a general phenomenon of the observed rod-sphere mixture.

DY 55.8 Thu 15:00 Poster B2

Stochastic rotor engine based on the electron shuttling mechanism — •Christopher W. Wächtler[1], Philipp Strasberg[2], and Gernot Schaller[1] — [1]Institute of Theoretical Physics, Berlin, Germany — [2]Física Teòrica: Informació i Fenòmens Quàntics, Barcelona, Spain

The single electron shuttle is an example of a nano-scale system exhibiting a transition towards self-oscillation, where mechanical oscillations of a metallic grain are achieved by sequential electron tunnelling between the grain and two connecting leads. We theoretically investigate how one can use this shuttling mechanism to build a stochastic rotor engine which converts between chemical and mechanical work by applying a bias voltage between the two leads. Furthermore, we show that this rotor engine can also be used as a heat engine by applying a temperature bias between the electronic leads and the heat reservoir connected to the rotor. Besides the average thermodynamic quantities we additionally study the fluctuations of these quantities.

DY 55.9 Thu 15:00 Poster B2

A generalization of the thermodynamic uncertainty relation to periodically driven systems — •Timur Koyuk[1], Udo Seifert[1], and Patrick Pietzonka[1,2] — [1]II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany — [2]DAMTP, Centre for Mathematical Sciences, University of Cambridge, CambridgeCB3 0WA, United Kingdom

The thermodynamic uncertainty relation expresses a universal tradeoff between precision and entropy production, which applies in its original formulation to current observables in steady-state systems. We generalize this relation to periodically time-dependent systems and, relatedly, to a larger class of inherently time-dependent current observables [1]. In the context of heat engines or molecular machines, our generalization applies not only to the work performed by constant driving forces, but also to the work performed while changing energy levels. The entropic term entering the generalized uncertainty relation is the sum of local rates of entropy production, which are modified by a factor that refers to an effective time-independent probability distribution. The conventional form of the thermodynamic uncertainty relation is recovered for a time-independently driven steady state and, additionally, in the limit of fast driving. We illustrate our results for a simple model of a heat engine with two energy levels.

[1] T. Koyuk, U. Seifert, and P. Pietzonka, A generalization of the thermodynamic uncertainty relation to periodically driven systems, J. Phys. A: Math. Theor. (2018), arXiv:1809.02113, in press.

DY 55.10 Thu 15:00 Poster B2

Unravelling the energetics of stochastic surface growth with artificial neural networks — •Thomas Martynec[1], Stefan Kowarik[2], and Sabine H.L. Klapp[1] — [1]Institut fuer Theoretische Physik, Technische Universitaet Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — [2]Institut fuer Physik, Humboldt-Universitaet zu Berlin, Newtonstrasse 15, 12489 Berlin, Germany

Stochastic surface growth by means of molecular beam epitaxy (MBE) is one of the most widely used techniques to fabricate thin film devices for various technological applications. It involves a competition between the adsorption of particles and various diffusion processes. Initially, particles like atoms, colloids or organic molecules are adsorbed on an ideally flat and defect free discrete substrate at rate F. This is followed by thermally activated Arrhenius-type diffusion processes to neighboring lattice sites. Once clusters are formed, nucleation on top of these clusters sets in. Depending on the strength Ees of the Ehrlich-Schwoebel barrier that reduces the interlayer transport rate of particles, surface growth proceeds either in a smooth or rough fashion. We demonstrate that an artificial neural network can precisely determine the value of the interlayer transport barrier from images of the growing islands with a 'wedding cake' morphology.

[1] C. M. Bishop, Rev. Sci. Instr. 65 1803 (1994)
[2] T.Martynec and S.H.L. Klapp Phys. Rev. E 98, 042801 (2018)

DY 55.11 Thu 15:00 Poster B2

The role of interactions in a in a quantum heat pump for fermionic atoms — •Manuel Alamo, Arko Roy, and Andre Eckardt — Max-Planck-Institut für Physik komplexer Systeme

We design and investigate a quantum heat pump for fermionic atoms in a structured optical potential. It is based on a structure given by two quantum dots hosting two levels each. By applying periodic driving, we engineer an energy-selective transport between both dots. Coupling each of them to a different fermionic reservoir, particles and heat is transported. We investigate the role of interactions on the performance of this device as a heat pump by employing Floquet-Born-Markov theory.

DY 55.12 Thu 15:00 Poster B2

Non-equilibrium dynamics of open systems exchanging particles — •JunHyuk Woo[1], Segun Goh[2], Jean-Yves Fortin[3], and MooYoung Choi[1] — [1]Department of Physics and Center for Theoretical Physics, Seoul National University, Seoul 151-747, Korea — [2]Institut für Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf, Germany — [3]Institut Jean Lamour, Groupe de Physique Statistique, Département de Physique de la Matière et des Matériaux, CNRS-UMR 7198, Vandoeuvre-lès-Nancy, F-54506, France

We consider an open system in contact with a reservoir, where particles as well as energies can be exchanged between them, and present a description of the dynamics in terms of mixed (pseudo)spin and state variables. Specifically, a master equation is constructed out of the exchange rates for particles and for energies, which allows us to probe the system in the grand canonical description. In particular, by means of the state resummation analysis, we obtain coupled time evolution equations for the probability distributions of the system as well as the environment. This is exemplified by a standard growth model, where the steady-state density function exhibits power-law behavior with the exponent depending on the microscopic parameters of the rate equations.

DY 55.13 Thu 15:00 Poster B2

Diffusion of solitons — •Tony Albers and Günter Radons — Institute of Physics, Chemnitz University of Technology, Chemnitz, Germany

Solitons propagating in nonlinear dissipative media have properties different from the ones in conservative media. One of the special features of these solitons are explosions, i.e., transient enlargements of the soliton that can lead to a spatial shift of the center of mass of the soliton if the explosion is asymmetric. A long sequence of such asymmetric explosions leads to a random walk of the soliton which is reminiscent of a diffusion process [1,2]. In this contribution, we use a simple but prototypical model, namely the one-dimensional cubic-quintic complex Ginzburg-Landau equation, to investigate the dynamical behavior of the solitons. We will characterize the random motion with quantities known from diffusion theory and, especially, we will pay attention to the ergodic properties of the soliton motion. We introduce two stochastic models, one discrete in time and one continuous in time, which are able to reproduce the observed features of the soliton motion.

[1] J. Cisternas, O. Descalzi, T. Albers, and G. Radons, Phys. Rev. Lett. **116**, 203901 (2016)
[2] J. Cisternas, T. Albers and G. Radons, Chaos **28**, 075505 (2018)

DY 55.14 Thu 15:00 Poster B2

Nonlinear response theory in classical systems — •Fenna Müller and Matthias Krüger — Institut für Theoretische Physik, Friedrich-Hund-Platz 1, 37077 Göttingen

The fluctuation-dissipation theorem describes the linear response of a system in relation to equilibrium fluctuations. However, there is

no corresponding general theorem or scheme to do the same for the nonlinear response. Here, we develop a coarse grained scheme for computation of nonlinear responses based on path integrals [2]. Comparing the time reversed system to its original, one can identify several components, such as entropy flux in the first order, as done e.g. in [1]. In experiments it is oftentimes impossible or impractical to observe the whole system with all its microstates, however. Therefore, we extend the path integral formalism to include a coarse graining, see [2]. All response formula describe the system in terms of coarse grained variables and direct access to microscopic variables is not necessary. We explore using this method for time dependent pertubations by applying it to the analytically solvable two state model.

[1] Basu, U., Krüger, M., Lazarescu, A., & Maes, C. (2015). Frenetic aspects of second order response. Physical Chemistry Chemical Physics, 17(9), 6653-6666. [2] Basu, U., Helden, L., & Krüger, M. (2018). Extrapolation to Nonequilibrium from Coarse-Grained Response Theory. Physical review letters, 120(18), 180604.