# DY 3: Statistical Physics 1 - organized by Barbara Drossel (Darmstadt), Sabine Klapp (Berlin) and Thomas Speck (Mainz)

Time: Monday 9:00–10:40 Location: DYb

DY 3.1 Mon 9:00 DYb

**The Five Problems of Irreversibility*** — •Michael te Vrugt — Institut für Theoretische Physik, Center for Soft Nanoscience, Westfälische Wilhelms-Universität Münster, D-48149, Münster, Germany

Macroscopic thermodynamics has a clear arrow of time: Systems irreversibly approach equilibrium accompanied by a monotonous increase of entropy. This stands in contrast to the laws of microscopic theories, which are invariant under time-reversal. The question how this difference can be explained has created a long debate, with suggestions involving coarse-graining methods as well as cosmological considerations about the entropy of the early universe. In this talk, I will show that a part of the difficulty in solving the problem of irreversibility arises from the fact that it actually consists of five different sub-problems [1], which are mixed in most discussions. Understanding why these problems have to be distinguished and how they are related to each other then allows to solve them on the basis of modern nonequilibrium statistical mechanics. The general approach is illustrated using the example of dynamical density functional theory (DDFT) [2].

[1] M. te Vrugt, arXiv:2004.01276 (2020)

[2] M. te Vrugt, H. Löwen, and R. Wittkowski, Advances in Physics 69, 121-247 (2020)

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DY 3.2 Mon 9:20 DYb

**Thermodynamic Uncertainty Relation for Time-Dependent Driving** — •Timur Koyuk and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Thermodynamic uncertainty relations yield a lower bound on entropy production in terms of the mean and fluctuations of a current. In this talk we will present the general form of the thermodynamic uncertainty relation for systems under arbitrary time-dependent driving from arbitrary initial states [1]. This approach unifies earlier derived relations valid for discrete Markovian systems or continuous overdamped Langevin systems. One powerful application of the TUR is to infer entropy production by observing an arbitrary current and its fluctuations without knowing the details of the interactions or underlying topology of the network. In this context we will extend the TUR beyond currents to state variables, which allows one to estimate entropy production by only observing, e.g., a binary observable. We will illustrate the quality of the bounds for various types of observables for the dynamical unfolding of a small protein, which is based on extant experimental data. As another important application of the TUR we will show how to bound the efficiency of cyclic heat engines by using the TUR for periodically driven systems [2]. This bound on the efficiency involves the output power, its fluctuations as well as its response with respect to the driving frequency. It thus imposes fundamental constraints on every cyclic stochastic heat engine for reaching Carnot efficiency.

[1] T. Koyuk and U. Seifert, Phys. Rev. Lett. 125, 260604 (2020).

[2] T. Koyuk and U. Seifert, Phys. Rev. Lett. 122, 230601 (2019).

DY 3.3 Mon 9:40 DYb

**Thermodynamic Uncertainty Relation for a Stochastic Field Theory – KPZ-Equation as a Paradigmatic Example** — •Oliver Niggemann and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart

Recently, a thermodynamic uncertainty relation (TUR) for a generic stochastic field theory has been proposed [1]. In this talk, I will first formulate a framework which describes the constituents of the field-theoretic TUR, namely current, entropy production and diffusivity. This general setting is then applied to the $(1+1)$-dimensional Kardar-Parisi-Zhang (KPZ) equation, a paradigmatic example of a non-linear field-theoretic Langevin equation. In particular, I will treat the dimensionless KPZ-equation with an effective coupling parameter, $\lambda_{\text{eff}}$, measuring the strength of the non-linearity. It will be shown that the field-theoretic TUR holds both in the weak and strong coupling regimes and that its value depends on $\lambda_{\text{eff}}$ [2]. For $\lambda_{\text{eff}} \downarrow 0$, the TUR product is equal to 5, whereas for $\lambda_{\text{eff}} \gg 1$ it grows linearly with $\lambda_{\text{eff}}$. There is no value for $\lambda_{\text{eff}}$ with the TUR product being saturated. Furthermore, I will present numerical simulations of the TUR constituents and the TUR product itself. These simulations display good agreement with the theoretical results for both the weak and strong coupling regime.

[1] Niggemann, O. and Seifert, U. *J Stat Phys* 178, 1142–1174 (2020). https://doi.org/10.1007/s10955-019-02479-x

[2] Niggemann, O. and Seifert, U. *J Stat Phys* 182, 25 (2021). https://doi.org/10.1007/s10955-020-02692-z

DY 3.4 Mon 10:00 DYb

**Entropy Production in Open Systems: The Predominant Role of Intraenvironment Correlations** — •Krzysztof Ptaszyński[1] and Massimiliano Esposito[2] — [1]Institute of Molecular Physics, Polish Academy of Sciences, Mariana Smoluchowskiego 17, 60-179 Poznań, Poland — [2]Complex Systems and Statistical Mechanics, Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg, Luxembourg

We show [1] that the entropy production in small open systems coupled to environments made of extended baths is predominantly caused by the displacement of the environment from equilibrium rather than, as often assumed, the mutual information between the system and the environment. The latter contribution is strongly bounded from above by the Araki-Lieb inequality, and therefore is not time-extensive, in contrast to the entropy production itself. Furthermore, we show that in the thermodynamic limit the entropy production is associated mainly with generation of the mutual information between initially uncorrelated environmental degrees of freedom. We confirm our results with exact numerical calculations of the system-environment dynamics.

[1] K. Ptaszyński, M. Esposito, Phys. Rev. Lett. 123, 200603 (2019)

DY 3.5 Mon 10:20 DYb

**Negative entropy production rates in Drude-Sommerfeld metals** — Marcus V. S. Bonança[1], •Pierre Nazé[1], and Sebastian Deffner[2,1] — [1]Universidade Estadual de Campinas, Campinas, Brazil — [2]University of Maryland, Baltimore County, Baltimore, USA

It is a commonly accepted creed that in typical situations the rate of entropy production is non-negative. We show that this assertion is not entirely correct if a time-dependent, external perturbation is not compensated by a rapid enough decay of the response function. This is demonstrated for three variants of the Drude model to describe electrical conduction in noble metals, namely the classical free electron gas, the Drude-Sommerfeld model, and the Extended Drude-Sommerfeld model. The analysis is concluded with a discussion of potential experimental verifications and ramifications of negative entropy production rates.

References:

[1] Marcus V. S. Bonança, Pierre Nazé, and Sebastian Deffner, Phys. Rev. E 103, 012109 (2021)