DY 23: Stochastic Thermodynamics

Time: Wednesday 9:30–13:00 Location: BH-N 128

DY 23.1 Wed 9:30 BH-N 128

Entropy production and thermodynamic inference for stochastic swimmers — •Michalis Chatzittofi[1], Jaime Agud-Canalejo[1], and Ramin Golestanian[1,2] — [1]Max Planck Institute for Dynamics and Self-Organization, Goettingen, Germany — [2]University of Oxford, Oxford, Germany

The question of characterization of the degree of non-equilibrium activity in active matter systems is studied in the context of a stochastic microswimmer model driven by a chemical cycle. The resulting dynamical properties and entropy production rate unravel a complex interplay between the chemical and the hydrodynamic degrees of freedom beyond linear response, which is not captured by conventional phenomenological approaches. By studying the precision-dissipation trade-off, a new protocol is proposed in which microscopic chemical driving forces can be inferred experimentally. Our findings highlight subtleties associated with the stochastic thermodynamics of autonomous microswimmers.

DY 23.2 Wed 9:45 BH-N 128

An estimator of entropy production for partially accessible Markov networks based on the observation of blurred transitions — •Benjamin Ertel and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

A central task in stochastic thermodynamics is the estimation of entropy production for partially accessible Markov networks as these models correspond to the partial observation of real-world systems. We establish an effective transition-based description for partially accessible Markov networks with transitions that are not distinguishable and therefore blurred for an external observer. We demonstrate that, in contrast to the description of fully resolved transitions, this effective description is non-Markovian at any point in time. We derive an information-theoretic bound for this non-ideal observation scenario which reduces to an operationally accessible entropy estimator under specific conditions that are met by a broad class of systems. We illustrate the operational relevance of this system class and the quality of the corresponding entropy estimator based on the numerical analysis of various representative examples.

DY 23.3 Wed 10:00 BH-N 128

Fluctuating Entropy Production on the Coarse-Grained Level: Inference and Localization of Irreversibility — •Jann van der Meer, Julius Degünther, and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Stochastic thermodynamics provides the framework to analyze thermodynamic laws and quantities along individual trajectories of small but fully observable systems. If the observable level fails to capture all relevant degrees of freedom, some form of effective, coarse-grained dynamics naturally emerges for which the principles of stochastic thermodynamics generally cease to be applicable straightforwardly. Our work unifies the notion of entropy production along an individual trajectory with that of a coarse-grained dynamics by establishing a framework based on snippets and Markovian events as fundamental building blocks. A key asset of a trajectory-based fluctuating entropy production is the ability to localize individual contributions to the total entropy production in time and space. As an illustration and potential application for inference we introduce a method for the detection of hidden driving. The framework applies equally to even and odd variables and, therefore, includes the peculiar case of entropy production in underdamped Langevin dynamics.

DY 23.4 Wed 10:15 BH-N 128

Thermodynamic cost for precision of general counting observables — •Patrick Pietzonka[1,2] and Francesco Coghi[3] — [1]School of Physics and Astronomy, University of Edinburgh, United Kingdom — [2]Max Planck Institute for the Physics of Complex Systems, Dresden, Germany — [3]Nordita, KTH Royal Institute of Technology and Stockholm University, Sweden

We analytically derive universal bounds that describe the trade-off between thermodynamic cost and precision in a sequence of events related to some internal changes of an otherwise hidden physical system. The precision is quantified by the fluctuations in either the number of events counted over time or the times between successive events. Our results are valid for the same broad class of nonequilibrium driven systems considered by the thermodynamic uncertainty relation, but they extend to both time-symmetric and asymmetric observables. We show how optimal precision saturating the bounds can be achieved. For waiting time fluctuations of asymmetric observables, a phase transition in the optimal configuration arises, where higher precision can be achieved by combining several signals.

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DY 23.5 Wed 10:30 BH-N 128

Thermodynamic cost of stochastic resetting — •Kristian S. Olsen[1], Deepak Gupta[2], Francesco Mori[3], and Supriya Krishnamurthy[4] — [1]Institut für Theoretische Physik II - Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Nordita, Royal Institute of Technology and Stockholm University, Sweden — [3]Rudolf Peierls Centre for Theoretical Physics, University of Oxford, Oxford, United Kingdom — [4]Department of Physics, Stockholm University, Sweden

Stochastic resetting gives rise to non-equilibrium steady states, and is known to appear in a wide range of both natural and man-made systems. Recent experiments have implemented resetting by means of an external trap, whereby a particle relaxes to the minimum of the trap and as such is reset in a finite time. Here we present a framework able to fully characterise the thermodynamic work of such resetting protocols. Our results are valid for a wide range of system, with the only assumption being that of relaxation to equilibrium in the resetting trap. Optimal trap shapes that minimise the work are studied for the case of Brownian motion.

DY 23.6 Wed 10:45 BH-N 128

Decoding sample-to-sample fluctuations in the time-ordering of non-Markovian sample paths — •Felix Tippner and Aljaz Godec — Max Planck Institute for Multidisciplinary Sciences, Göttingen, Germany

Inherent to almost all measurements is the loss of information as only a small number of degrees of freedom can be simultaneously observed. These measurements track projections of higher dimensional stochastic processes. Besides introducing (or enhancing) non-Markovian effects, such projections often hide features like irreversible currents (i.e., driven vs. non-driven) or barriers in the energy landscape. By studying correlations and comparing (systematic) sample-to-sample fluctuations of path-wise observables, such as empirical densities and currents inferred from projected trajectories—which may correspond, e.g., to time series of single-molecule measurements—we are able to gain qualitative insight into the aforementioned hidden features that cannot be observed upon ensemble averaging.

DY 23.7 Wed 11:00 BH-N 128

Nonequilibrium fluctuations of chemical reaction networks at criticality — •Benedikt Remlein and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Chemical reaction networks can undergo nonequilibrium phase transitions upon variation of external control parameters like the chemical potential of one species. We investigate the critical fluctuations of the flux in the associated chemostats, which is proportional to the entropy production, for two paradigmatic models, the Schlögl model and the Brusselator. In both cases, numerical simulations show that the corresponding diffusion coefficient diverges at the critical point as a function of system size albeit with different exponents. In the vicinity of the transition, the diffusion coefficient in the Schlögl model follows a scaling form. We develop an analytical approach based on van Kampen's system size expansion that yields these exponents. For the Brusselator model, we numerically find that the diffusion coefficient as function of the control parameter develops a discontinuity while increasing the system size.

15 min. break

DY 23.8 Wed 11:30 BH-N 128

Thermodynamically efficient agents — •Paul C. Barth, Lukas

J. Fiderer, Isaac D. Smith, Marius Krumm, Fulvio Flamini, and Hans J. Briegel — Institute for Theoretical Physics, University of Innsbruck, 6020 Innsbruck, Austria

Landauer's bound and its generalizations such as the information-processing second law provide energetic limits not only on information erasure but also on pattern manipulation and computations in general. In this work, we generalize these bounds further to account for agents which interact with an environment via a percept-action loop. Within our framework, we then design and analyze toy environments and thereby demonstrate that efficient agents, which maximize work production, do not always adhere to zero entropy production. Furthermore, we introduce a thermodynamic framework for learning by leveraging similarities between maximum work extraction and reward maximization in reinforcement learning. We apply this framework to an existing reinforcement learning scheme, namely projective simulation. We also discuss a possible quantization of our framework. This line of research promises new insights into the energetic aspects of adaptive behavior in natural and artificial system.

DY 23.9 Wed 11:45 BH-N 128

Thermodynamically consistent model of an active Ornstein-Uhlenbeck particle — •Jonas Fritz and Udo Seifert — II. Institut für Theoretische Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Identifying the full entropy production of active particles is a challenging task. We introduce a microscopic, thermodynamically consistent model that leads to active Ornstein-Uhlenbeck statistics in the continuum limit [1]. Our minimal model consists of a particle with a fluctuating number of active reaction sites which contribute to its active self-propulsion on a lattice. In addition, the model also takes ordinary thermal noise into account. This approach allows us to identify the full entropy production stemming from both thermal diffusion and active driving. Extant methods based on the comparison of forward and time-reversed trajectory underestimate the physical entropy production when applied to the Langevin equations obtained from our model. Constructing microscopic Markovian models can thus provide a benchmark for determining the entropy production in non-Markovian active systems.

[1] Jonas H. Fritz and Udo Seifert, J. Stat. Mech. (2023) 093204

DY 23.10 Wed 12:00 BH-N 128

Thermodynamics of active matter: Tracking dissipation across scales — •Robin Bebon, Joshua F. Robinson, and Thomas Speck — Institute for Theoretical Physics 4, University of Stuttgart, Heisenbergstraße 3, 70569 Stuttgart, Germany

The non-equilibrium "active" nature of living systems becomes manifest in the spatial and temporal organization of hierarchical structures, which provide essential functionality. Maintaining activity is necessarily coupled to continual energy consumption, which in turn posits dissipation as the central constraint of any such process. Here we derive exact expressions for the dissipation rate of catalytically propelled active particles, ranging across length scales from individual agents to large-scale collectives. Commencing from a microscopic model of a single catalytic particle that interacts with explicit solute molecules, we motivate a mesoscopic many-body description reminiscent of active Brownian particles. Through further coarse-graining, we obtain a macroscopic field theoretic description based on effective hydrodynamic equations and sketch how to treat scalar field theories. This systematic bottom-up construction enables precise bookkeeping of the degrees of freedom that partake in the stochastic energetics and shows that dissipation is, both locally and globally, accompanied by a continual solute flux between solute reservoirs. We employ our results to gain insights into the thermodynamic footprint of confinement and the role of dissipation in motility-induced phase separation. Moreover, we demonstrate how the phenomenological framework of linear irreversible thermodynamics unfolds from our microscopic approach.

DY 23.11 Wed 12:15 BH-N 128

Active matter under control — Luke K. Davis[1,2], Karel Proesmans[1,3], and •Etienne Fodor[1] — [1]Department of Physics and Materials Science, University of Luxembourg, L-1511 Luxembourg — [2]Department of Mathematics, University College London, 25 Gordon Street, London, England — [3]Niels Bohr International Academy, Niels Bohr Institute, University of Copenhagen, Blegdamsvej 17, 2100 Copenhagen, Denmark

Active constituents burn fuel to sustain individual motion, giving rise to collective effects that are not seen in systems at thermal equilibrium. There is a great potential in harnessing the striking phenomenology of active matter to build novel controllable and responsive materials that surpass passive ones. Yet, we currently lack a systematic roadmap to predict the protocols driving active systems between different states in a way that is thermodynamically optimal. Equilibrium thermodynamics is an inadequate foundation to this end, due to the dissipation rate arising from the constant fuel consumption in active matter. Here, we derive and implement a versatile framework for the thermodynamic control of active matter. Combining recent developments in stochastic thermodynamics and nonequilibrium response theory, our approach shows how to find the optimal control for either continuous- or discrete-state active systems operating arbitrarily far from equilibrium. Our results open the door to designing novel active materials which are not only built to stabilize specific nonequilibrium collective states, but are also optimized to switch between different states at minimum dissipation.

DY 23.12 Wed 12:30 BH-N 128

Optimizing the Energetics of the Finite-time Driving of Field Theories — •Atul Tanaji Mohite — Universität des Saarlands

Field theories have been extremely successful in characterizing the universal properties of various phase transitions, and in delineating a few canonical models which capture the essential Physics at play in a large class of systems. Interestingly, a generic framework for optimizing the energetic cost associated with the finite-time driving of such systems is still largely missing. Here, building on recent advances in stochastic thermodynamics and optimal transport theory, we show how to analytically derive the optimal driving protocols that minimize work, which we apply to cases with either conserved or non-conserved scalar order parameters in the weak noise regime. Moreover, we formulate a numerical multi-optimization problem to simultaneously optimize the mean and variance of work, leading to revealing a first-order phase transition in the corresponding Pareto front, which features the coexistence of multiple optimal protocols. Overall, our results elucidate how to drive field dynamics at a minimal energetic cost, with the potential to be deployed in a broad class of systems.

DY 23.13 Wed 12:45 BH-N 128

Geometrically frustrated systems which are as singles hotter than in company — •Wolfgang Bauer — Dept. of Internal Medicine I, UKW, Würzburg, Germany

Systems of same temperature, which are brought from initial isolation to weak thermal coupling, maintain their temperature, which is equivalent to that of the combined system. Any other scenario would be in conflict with our notion of thermal stability and the 2nd law of thermodynamics. Special geometrically frustrated systems (GFSs), which are constraint to reside at negative Boltzmann temperature, challenge the above notion. When brought in weak thermal contact, the assembly of GFSs is in equilibrium cooler than its constituents, and may even exhibit positive Boltzmann temperatures. The 2nd law of thermodynamics would imply heat flow related to the gradient of Boltzmann temperatures between a single GFS and the residual assembly under equilibrium conditions. This conflict is resolved by considering the canonical temperature of a GFS, derived from information theory, which differs from its Boltzmann temperature. We show, that the gradient of Boltzmann temperatures predicts the stochastic drift of the most probable state of a GFS within its environment, whereas the canonical temperature gradient defines the direction of heat flow, which restores the 2nd law of thermodynamics.