Stochastic Thermodynamics: Experiment and Theory

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Introduction

Stochastic thermodynamics describe the non-equilibrium behavior of mesoscopic physical systems and has emerged as a well-defined subfield of statistical physics during the last few decades. Nowadays, there exists a vibrant community of statistical physicists working in stochastic thermodynamics. While much of the initial progress in this field was theoretical or focused on thought experiments such as the celebrated Maxwell demon, impressive technological advances in recent years have enabled tests of many of the fundamental principles.

The workshop *Stochastic Thermodynamics: Experiment and Theory*, held at the Max-Planck Institute for Complex Systems in Dresden, 10–14 September 2018 had as primary goal to bring together theorists and experimentalists to discuss the state of the art in stochastic thermodynamics and the main future challenges. The workshop was characterized by a vibrant atmosphere, with participants from all over the world sharing their views on the latest results and the outstanding open questions in this field. Many of these discussions have resulted in novel collaborations and significant steps forward.

This special edition of *Journal of Statistical Mechanics: Theory and Experiment* collects the outcome of these discussions.

1. The articles

1.1. Connecting to experiments

- Saha and Marathe discuss work extraction from an engine that is constructed using a harmonic potential with modulated stiffness, where the system is in contact with a conventional heat bath for half the cycle and in contact with an active bath (modeled by an Ornstein-Uhlenbeck process) for the second half of the cycle. In certain regimes, such an engine can be more efficient than a similar two-temperature heat engine. [1]

- Monnet et al. generalize Nyquist's 1928 expression for the voltage fluctuations across a resistor at constant temperature (Johnson noise) to the case of a resistor whose two ends contact two thermal reservoirs with different temperatures. Experiments agree with a simple theory that predicts that in a nonequilibrium steady state, the fluctuations are equivalent to an equilibrium system held at the mean temperature of the two thermostats. [2]
- Severino et al. give a detailed account of how to measure equilibrium free-energy differences between folded and unfolded states of single molecules (DNA and RNA hairpins). In particular, they give a careful treatment of how to eliminate systematic contributions from the elastic stretching of the tethers holding the molecule of interest. These can contribute large systematic errors and must be accounted for correctly in order to infer accurate free-energy estimates. [3]
- Gaspard and Kapral study the intriguing phenomenon of self-thermo-phoresis for a Janus particle coated with a light-absorbing film on one half. When the particle is illuminated, a temperature gradient induces spontaneous motion. The authors give a thermodynamically consistent derivation of Langevin equations for the particle motion, starting from the level of fluctuating hydrodynamics. Their predictions call for future experimental tests. [4]
- Maes and Netocny discuss how to generalize heat-capacity measurements to systems in a nonequilibrium steady state. The central result is that a harmonic modulation can be used to isolate the small contribution of a nonequilibrium heat capacity, in a way that can be implemented experimentally. Such result is expected to provide novel insights on the characterization of the change in a material's thermal properties when driven away from equilibrium. [5]

1.2. New universal fluctuations

- Hartich and Godec develop a formalism relating relaxation and first-passage time statistics of Markovian stochastic processes. They prove that the timescales at which a particle is absorbed by a target interlace with the corresponding relaxation timescales. This duality allows them to determine exactly the first-passage time distribution from the relaxation spectra. Notably, they apply this technique to provide the first exact derivation of the first-passage-time distribution for an Ornstein-Uhlenbeck process. [6]
- Chétrite et al. provide encyclopedic knowledge on a collection of relevant information-theoretic measures of stochastic systems with and without bipartite structure. The authors provide a general formalism describing a collection of information measures (learning rates, transfer entropy, etc) for continuous-time stochastic processes, deriving exact results for diffusion processes with multiplicative noise. The general theory is illustrated with examples of stochastic processes relevant in physics and biology. [7]
- Neri et al. demonstrate an integral fluctuation theorem at stopping times and discuss its physical interpretation and consequences. This theorem is a remarkable

extension of the traditional integral fluctuation theorem and results from the fact that the stochastic entropy production in nonequilibrium stationary processes is an exponential martingale. Implications of this result are discussed in the context of new universal fluctuations of entropy production such as first-passage statistics and extreme values. An important consequence of the work is the fact that heat engines stopped at a cleverly chosen time can surpass Carnot's efficiency. [8]

- Derivaux and De Decker study coupled transport of heat and matter at the mesoscopic scale, within the extended local equilibrium framework. They study distribution of two types of efficiency (separation and thermodynamic efficiencies) in this process, and in particular the condition for having a bimodal distribution of efficiency. Theoretical results are supplemented by a vast amount of numerical simulations which highlight the universality of the theory, applicable also to stochastic efficiencies of ratios of dissipations used in Carnot cycles or the ratio of electrical and heat fluxes in fuel cells. [9,10]

1.3. Thermodynamic uncertainty relations

- Barato and coworkers present a number of different thermodynamic uncertainty relations, differing in the underlying hypothesis and including generalizations out of steady state. They show how these different results can be placed in a unified theoretical framework. In particular, their results apply to a broad class of functionals of stochastic trajectories that are linear combinations of the empirical flow and densities, valid for time-periodic Markov chains with continuous time. Applications of these results to experiments range from artificial molecular pumps to colloidal heat engines. [11]
- Proesmans and Horowitz extend thermodynamic uncertainty relations to systems with broken time-reversal symmetry. Such systems arise when magnetic fields are present and in otherwise time-symmetric systems that are driven by fields that are not invariant under time reversal. They derive explicit bounds on the amount of dissipation required to suppress fluctuations in the hysteresis of currents (sum of current in forward and time-reversed system). [12]
- Vroylandt et al. discuss trade-offs between power and efficiency for thermodynamic machines at steady states. They show that these trade-offs must satisfy several inequalities, some of which are related with thermodynamic uncertainty relations. Key results include bounds on the entropy production for thermal machines in terms of the degree of coupling between its input and output energy sources and a a hierarchy of power-efficiency trade-offs which are tested with stochastic models of molecular motors. [13]

1.4. Adding rigor

- Mandaiya and Khaymovich review many versions of fluctuation theorems that have been among the key advances of stochastic thermodynamics and then introduce new relations between their finite-time and infinite-time versions. These relations clarify surprising connections between fluctuation relations and topics such as first-passage-time distributions and the fluctuations of waveforms near the Anderson localization transition. [14]

- Bo, Lim, and Eichhorn add rigor to the justification of the commonly used Stratonovich convention in evaluating discretized, path-dependent stochastic quantities such as heat and work. Starting from generalized Langevin dynamics driven by noise with a finite time correlation, they carefully consider the white-noise and small-mass limits to arrive at the commonly used overdamped expressions. They also clarify some anomalies in the evaluation of entropy production. [15]
- Das and Gupta thoroughly study, with theory and numerical simulations, a model of classical Heisenberg spins with long-range interactions relaxing towards thermal equilibrium. Using this model, the authors unequivocally establish that quasi-stationarity observed in deterministic dynamics of long-range-interacting systems is washed away by fluctuations induced through contact of the system with an environment. The work highlights the ubiquity of a phenomenon—absence of quasi-stationarity in stochastic dynamics—that had been reported earlier only in single-particle dynamics. [16]
- Busiello and Maritan compare the entropy production rate of a Master equation with that of a Fokker-Planck equation derived from it via a diffusion approximation. They discuss the discrepancy between the two approaches and how it can be resolved. In particular, they propose a new coarse-graining procedure different to Kramers-Moyal which ensures the least information loss when taking the diffusive limit. [17]

Finally, we dedicate a special mention to the delightful oral presentation of Christian Maes on the ventures and misadventures of Th. Smiths (The "Statistical mechanician in the street") as he wrestles with developing a more intuitive understanding of the role of thermodynamics for problems in cosmology—the horizon problem, flatness, information paradox, dark-energy puzzle, and more.

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List of participants

The list of participants included some of the major researchers that have played a seminal role in the development of this field. The complete list is as follows: Janet Anders, Ricardo Arias-Gonzalez, John Bechhoefer, Clemens Bechinger, Ludovic Bellon, Alexander Blokhuis, Stefano Bo, Fredrik Brange, Daniel Maria Busiello, Raphael Chetrite, Davide Chiuchiu, Sergio Ciliberto, Livia Conti, Clara del Junco, Jean-Francois Derivaux, Luis Dinis, Ralf Eichhorn, Massimiliano Esposito, Etienne Fodor, Andre Fuchs, Ken Funo, Pierre Gaspard, Momcilo Gavrilov, Todd Gingrich, Shamik Gupta, Peter Hanggi, David Hartich, Patrick Hofer, Jordan Horowitz, Christopher Jarzynski, Frank Julicher, Timo Kerremans, Ivan Khaymovich, David Lacoste, Jae Sung Lee, Zhiyue

Lu, Eric Lutz, Christian Maes, Olivier Maillet, Rahul Marathe, Ignacio A. Martínez, Antoine Naert, Izaak Neri, Karel Netocny, Basile Nguyen, Rui Pan, Govind Paneru, Jukka Pekola, Patrick Pietzonka, Simone Pigolotti, Matteo Polettini, Karel Proesmans, Krzysztof Ptaszynski, Haitao Quan, Somrita Ray, Oren Raz, Raul Rica, Felix Ritort, Juan MR Parrondo, Edgar Roldan, Martin Luc Rosinberg, Takahiro Sagawa, Arnab Saha, Shin-ichi Sasa, Udo Seifert, Ken Sekimoto, Naoto Shiraishi, Shilpi Singh, David Sivak, Shoichi Toyabe, Matthias Uhl, Suriyanarayanan Vaikuntanathan, Gatien Verley, and Hadrien Vroylandt.

One person who very much wanted to attend this workshop was Christian Van den Broeck. As a community, we mourn his passing. The activity and vitality of this workshop owed much to his pioneering and continuing research that helped to create and sustain the field of stochastic thermodynamics.

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