Finite-time time dynamical phase transition in entropy production rate?

Jan Meibohm and Sabine Klapp

Recently, finite-time dynamical transitions have become a focus of growing interest in both, classical statistical mechanics and in quantum systems. The present master project is concerned with the occurrence, and associated thermodynamic signatures, of finite-time time dynamical phase transitions in *nonequilibrium* classical systems under an external drive. Specifically, we will consider two paradigmatic model systems, namely a one-dimensional random walk with asymmetric rates, and a driven colloidal particle on a periodic potential. A key quantity of the investigations will be the time-dependent entropy production rate and its fluctuations. The project combines various concepts from non-equilibrium statistical physics including theory of stochastic processes, stochastic thermodynamics, and large deviation theory. The actual investigations involve analytical calculations based on stochastic differential equations and discrete Master equations, as well as corresponding numerical methods (stochastic simulations).

I. BACKGROUND

The analysis of entropy production has become a major theme of modern nonequilibrium statistical mechanics. Entropy production determines the irreversibility of a given process and thus provides a measure of how much a system departs from equilibrium. Within the theory of Stochastic Thermodynamics [5–7], thermodynamic observables, including entropy production, are fluctuating quantities with an associated probability distribution.

Entropy production is often studied in so-called nonequilibrium steady states. Similarly to steady states at equilibrium, nonequilibrium steady states are time-independent, but they have an associated finite entropy production rate

$$\sigma(t) = \frac{\Sigma(t)}{t}, \tag{1}$$

where Σ denotes the total (accumulated) entropy production and t denotes time. Although σ is a random variable in nonequilibrium steady states, it converges to a deterministic average value

$$\lim_{t\to\infty} \sigma(t) = \langle\sigma\rangle, \tag{2}$$

due to the law of large numbers. In other words, at long times, the fluctuations of $\sigma(t)$ become less and less important. However, at finite but large time, fluctuations of σ may still occur, due to extreme, but very unlikely events.

The probabilities for such extreme events typically scale exponentially in time [8] and one has for the probability distribution $P(\sigma)$,

$$P(\sigma) \propto \mathrm{e}^{-tI(\sigma)}, \tag{3}$$

where $I(\sigma)$ denotes the so-called rate function. The rate function $I(\sigma)$ quantifies the probability of exponentially unlikely, extreme events, thus generalising the central limit theorem.

The properties of the rate function away from the average value $\langle\sigma\rangle$, where $I(\langle\sigma\rangle) = 0$, teach us a lot about the extreme behaviour of a system. For this reason, the rate function of entropy production is frequently studied for nonequilibrium systems.

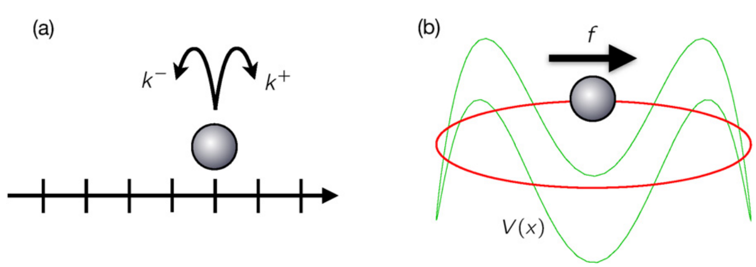

FIG. 1. Sketch of the models in the proposed study. (a) Discrete asymmetric random walk with transition rates $k^+ > k^-$. (b) Driven colloidal particle on a continuous ring with forcing f and potential $V(x)$. (Figure from Ref. [1])

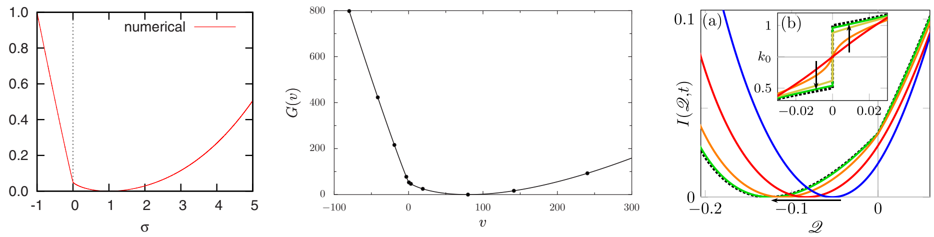

FIG. 2. Rate functions of entropy production in different models. (*Left*) Driven colloidal particle on a ring. (Figure from Ref. [2]). (*Middle*) Molecular motor model. (Figure from Ref. [3]). (*Right*) Relaxation of Curie-Weiss model. The rate function is smooth at short times (blue, red and orange) but develops a kink at longer times (green and black dashed). (Figure from [4]).

II. MODELS

We propose to study the rate function of entropy production in two models of nonequilibrium statistical mechanics, shown in Fig. 1. In both cases, non-equilibrium is induced externally, e.g., by a constant force.

The first model [Fig. 1(a)] is an asymmetric random walk on a one-dimensional lattice, described by a discrete Master equation. In this model, a random walker may jump to the right at rate k^+ and to left at rate k^-, where $k^+ > k^-$. Due to the difference in the transition rates, the random walker will, on average, move to the right. This average motion results in an average probability flux, associated with a finite entropy production rate.

The second model [Fig. 1(b)] is a continuous model for a driven colloidal particle on a ring. The particle experiences a periodic potential $V(x)$, but is driven in one direction by a force f. Similar to the first model, the driving f results in an average directed motion of the particle, and thus to a finite rate of entropy production.

The two models are intimately related: When the barriers of the periodic potential are large compared to the thermal energy, one may approximate the continuous motion by a (discrete) one-dimensional random walk with asymmetric rates [9, 10].

III. ENTROPY PRODUCTION AT FINITE TIME

The rate function for the models given in Sec. II have been studied by different authors [1, 2, 11, 12]. An interesting feature that has been noted is a remarkable kink in the rate function $I(\sigma)$ at $\sigma = 0$ for weak noise or strong driving, see left panel in Fig. 2. Similar kinks have also been observed in quite different models, e.g., in a model for a molecular model [3], see middle panel in Fig. 2. The kink in the rate function has been interpreted as a dynamical phase transition [11].

Dynamical phase transitions describe abrupt changes of the dynamics of a system as an external control parameter (here the entropy production) is altered. Dynamical phase transitions are nonequilibrium analogues of equilibrium phase transitions, and they thus give important insights into dynamical properties of a system. They occur in both, classical and quantum systems [13, 14].

Recently, a new class of dynamical phase transitions has been reported, so-called finite-time dynamical phase transitions [4, 15]. In contrast to conventional dynamical phase transitions, which occur in long-time rate functions obtained in nonequilibrium steady states, finite-time dynamical phase transitions form at a finite time.

In Ref. [4] the authors analysed the heat release $\mathscr{Q}$ (proportional $-\Sigma$) of a mean field magnet model. They found a time-dependent rate function $I(\mathscr{Q},t)$ that has a similar kink as $I(\sigma)$, see right panel of Fig. 2, at long (but finite) times, but that looks smooth at short times.

The question that arises from this analogy is if perhaps the dynamical phase transition for the particle on a ring, or for the asymmetric random walk, has also formed at finite time. If so, this would require a reinterpretation of the characterisation of the dynamical phase transition. What is often done to characterise dynamical phase transitions is to simply see if the derivative of the rate function changes continuously, or not. If if does, then the transition is said to be of second order, otherwise of first order.

Finite-time dynamical phase transitions, by contrast, allow the consistent definition of an order parameter, which changes continuously at second-order transitions [4, 15].

In addition to exploring the thermodynamics, we will also investigate relations to changes in the actual dynamics, such as transitions between diffusive and subdiffusive motion [9, 10].

IV. METHODS

The project is requires the application of a variety of different tools from statistical mechanics. The candidate will learn about methods as diverse as:

- stochastic differential equations
- discrete Master equations
- large deviation theory (the theory of rate events)
- instanton methods (optimal fluctuation theory)
- stochastic (Gillespie) simulations

All these methods have applications in a wide range of fields in- and outside of nonequilibrium statistical mechanics.

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