Fluctuation relations and fluctuation-response relations for molecular motors

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Abstract. Fluctuation relations are a set of remarkable relations obeyed by a large class of systems and arbitrarily far from equilibrium. It is interesting to discuss the implications of these relations for molecular motors, which are chemically driven enzymes. These enzymes operate stochastically at the molecular level and for these reasons undergo large thermal fluctuations. Using simple ratchet models of molecular motors, the various forms of fluctuation relations can be illustrated in a simple way. In the linear regime, finite time fluctuation relations imply specific modified fluctuation-dissipation relations.

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INTRODUCTION

In recent years, a renewed interest has arisen in ratchet models in the context of non-equilibrium statistical physics. There is large family of ratchet models, but only the isothermal models are relevant for molecular motors. In these models, the coupling of the ratchet to some external agent (e.g., a chemical reaction) continuously drives the system out of equilibrium, and this allows work to be extracted under certain conditions. There is no contradiction with thermodynamics here: the system is far from equilibrium and the ratchet plays the role of a transducer between the energy put in by the agent (e.g., chemical energy) and the mechanical work extracted. The analysis of the energetics of such devices far from equilibrium requires concepts that go beyond the classical laws of thermodynamics. The fluctuation relations, is one of such concepts. These relations, which hold arbitrarily far from equilibrium, can be seen as macroscopic consequences of the invariance under time reversal of the dynamics at the microscopic scale. It is interesting to apply these concepts to small systems such as molecular motors, which operate naturally far from equilibrium and undergo large thermal fluctuations.

As shown in [1], models of molecular motors can provide a particularly clear and pedagogical illustration of fluctuation relations, such as the Gallovotti-Cohen symmetry relation, which is known to hold generally for systems obeying markovian dynamics. This study has been carried out for both the discrete and for the continuous version of the model, called the flashing ratchet [2]. Interestingly, one finds that the Gallavotti-Cohen symmetry is no longer guaranteed if the system is not described by sufficiently variables to properly account for the reversibility of the microscopic dynamics. However, the symmetry can be restored in these models, when variables are added so as to render the dynamics markovian.

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LINEAR RESPONSE NEAR A NON-EQUILIBRIUM STEADY-STATE

Within the linear response regime and for slightly perturbed non-equilibrium steady states (Ness), finite time fluctuation relations, can be used to obtain modified fluctuation-response relations for systems obeying markovian dynamics [3, 4, 5]. These fluctuation-response relations qualify as extensions of the well-known fluctuation-dissipation theorem (FDT), because they hold in the vicinity of a non-equilibrium steady-state rather than near an equilibrium state as in the classic FDT.

Let us consider a system initially in non-equilibrium steady state, characterized by a (set of) control parameters denoted by λ. For a given value of λ, we assume that there exists a steady state with stationary probability distribution $P_{stat}(c,\lambda) = \exp(-\phi(c,\lambda))$. A time-dependent perturbation of the dynamics around the fixed value λ_0 will be described by $\lambda(s) = \lambda_0 + \delta\lambda(s)$ for $t > s$. The response $R(t,s) = \delta\langle A(c(t),\lambda_0)\rangle_{\text{path}}/\delta\lambda(s)$ of the dynamic observable A that depends on the microscopic configuration $c(t)$ at time t is given by the nonequilibrium FDT [3, 4]:

$$R(t,s) = -\frac{d}{ds}\left\langle \frac{\partial\phi(c(s),\lambda_0)}{\partial\lambda} A(c(t),\lambda_0) \right\rangle_0, \tag{1}$$

where $\langle..\rangle_0$ denotes the average in the stationary state with the control parameter λ_0. For thermal equilibrium, we have $\phi(c,\lambda) = \beta(H(c) - \lambda O(c) - F(\lambda))$, where H is the unperturbed hamiltonian, O is a perturbation, F is the free energy; and the usual form of the fluctuation-dissipation theorem is recovered from Eq. 1.

In Ref. [5], we have given a compact derivation of Eq. 1 and provided two applications: In the first application introduced in Ref. [6], a particle obeying overdamped Langevin dynamics is subjected to a periodic potential and a non-conservative force. In the second application, a discrete two-states ratchet model of a molecular motor is considered. In this case, the modified FDT takes the form of Green-Kubo relations characterizing the response of the motor near a NESS. We have observed that the modified FDT relation requires a knowledge of the relevant degrees of freedom in order to be able to distinguish an equilibrium state from a non-equilibrium steady state, just as it does for the existence of a Gallavotti-Cohen symmetry [2].

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