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Fluctuation theorems in inhomogeneous media under coarse graining

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ABSTRACT

We compare the fluctuation relations for work and entropy in underdamped and overdamped systems, when the friction coefficient of the medium is space-dependent. We find that these relations remain unaffected in both cases. We have restricted ourselves to Stratonovich discretization scheme for the overdamped case.

1. Introduction

The last couple of decades have observed a steadily growing interest in the field of systems at mesoscopic scales, thanks to the growing understanding of machines and engines with smaller dimensions. This has led to the area of stochastic thermodynamics which provides a framework for extending notions of classical thermodynamics to small systems wherein concepts of work, heat, and entropy are extended to the level of individual trajectories during nonequilibrium processes (ensembles). Research in this area has given birth to a group of exact and powerful theorems that dictate the behavior of such systems. They are commonly referred to as the *fluctuation theorems* (FTs) [1–17], and these theorems are valid even far from equilibrium, a feat that is beyond the scope of the well-established linear response theory. The theorems provide stringent restrictions on the probabilities of phase space trajectories in which second law is transiently "violated". They show that at the level where fluctuations are comparable to the relevant energy exchanges of the system, one needs to replace the associated quantities in the statement of the second law by their *averages*: $\langle W\rangle \geqslant \Delta F$ or $\langle \Delta s_{tot}\rangle \geqslant 0$ [9,13,14]. Here the angular brackets represent the ensemble average. Thus, they in essence uphold the second law, even at the mesoscopic level, however, for the average properties.

The Crooks Fluctuation theorem (CFT) for heat states that the ratio of the probabilities of forward trajectory and the corresponding reverse trajectory for given initial states is given by [15,16]

$$\frac{P[X|x_0]}{\tilde{P}[\tilde{X}|x_\tau]} = e^{\beta Q}. \tag{1}$$

Here, X is the short form of the phase space trajectory along the forward process $x_0, x_1, \dots, x_\tau$ generated by the protocol $\lambda(t)$. x_i represents the phase space point at time t_i. $\tilde{X}$ is the corresponding reverse trajectory generated by the time reversed protocol $\lambda(\tau - t)$, where τ is the time of observation. x_0 is a given initial state of the forward process. The reverse process begins from the state $\tilde{x}_\tau$, which is the time-reversal of the final state x_τ of the forward process.

Using CFT, several other theorems like the Jarzynski equality and entropy production FT can be easily derived [15,16].

In this paper, we study the validity of these FTs in the presence of coarse-graining, when we transform the underdamped Langevin equation to the overdamped one, in the limit of high friction. We find that a prominent difference in the analysis is observed between the overdamped (coarse-grained) and the underdamped systems, when the friction coefficient is space-dependent [18–21]. It should be noted that space-dependent friction does not alter the equilibrium state. However, Langevin dynamics of the system gets modified especially for the overdamped case. There are several physical systems wherein friction is space-dependent (see [21] and the references therein).

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2. Crooks theorem in presence of space-dependent friction

In the presence of space-dependent friction $\gamma(x)$, the equation of motion of the underdamped system of mass m moving in a time-dependent potential $U(x,t)$ is given by

$$m\dot{v} = -\gamma(x)v - U'(x,t) + \sqrt{2\gamma(x)T}\xi(t). \tag{2}$$

Note that the above equation contains multiplicative noise term. Here, T is the temperature of the bath, while $\xi(t)$ is the delta-correlated Gaussian noise with zero mean: $\langle\xi(t)\rangle = 0$; $\langle\xi(t)\xi(t')\rangle = \delta(t-t')$. The overhead dot denotes time-derivative, whereas prime represents space derivative. Eq. (2) has been derived microscopically by invoking system and bath coupling [19,20]. It is shown that the high damping limit of Eq. (2) is not equivalent to ignoring only inertial term [18–21]. The detailed treatment leads to an extra term that is crucial for system to reach equilibrium state in absence of time-dependent perturbations (see Eq. (19) below).

Roughly speaking, this happens in the overdamped case because the random forces $\xi(t)$ appear as delta-function pulses that cause jumps in x. It then becomes unclear what value of x must be provided in the argument of the function $\sqrt{2\gamma(x)T}$, because the value of the position at the time the delta-peak appears becomes undefined [22]. It does not converge to a unique value even in the limit of small time step Δt. In fact, we can plug in any value of position in-between $x(t)$ (position before the jump) and $x(t+\Delta t)$ (position after the jump). These different values of position lead to different discretization schemes. The case is simpler in case of underdamped Langevin equation. There, the jumps are caused in the velocities, while the position is a much smoother variable (being an integral over the velocities). In other words, it does not feel the noise as delta peaks, but instead as a more well-behaved function. In that case, in the limit of small Δt, the argument of g is given by the unambiguous value $x(t)$. Thus, in this case, an update in the values of x and v will be unique in each time step.

Let us now check the validity of CFT in both the underdamped and overdamped cases.

2.1. Underdamped case

At first we want to calculate the ratio of path probabilities between forward and reverse process. In a given process, let the evolution of the system in phase space be denoted by the phase space trajectory $X(t) \equiv \{x_0, x_1, \ldots, x_\tau\}$. Here, x_k represents the phase point at time $t = t_k$. In general, the phase point includes both the position and the velocity coordinates of the system. In the overdamped case, however, it would consist of the position coordinate only. Now, a given path $X(t)$, for a given initial point x_0, would be fully determined if the sequence of noise terms for the entire time of observation is available (this happens because there is no unambiguity in either the positions or the velocities, while updating their values by using the underdamped Langevin equation, as discussed above): $\boldsymbol{\xi} \equiv \{\xi_0, \xi_1, \ldots, \xi_{\tau-1}\}$. The probability distribution of ξ_k is given by

$$P(\xi_k) \propto e^{-\xi_k^2\,dt/2}. \tag{3}$$

Therefore, the probability of obtaining the sequence $\boldsymbol{\xi}$ will be [12,23]

$$P\big[\boldsymbol{\xi(t)}\big] \propto \exp\left[-\frac{1}{2}\int_0^\tau \xi^2(t)\,dt\right]. \tag{4}$$

Now, from the probability $P[\boldsymbol{\xi(t)}]$ of the path $\boldsymbol{\xi(t)}$ in noise space, we can obtain the probability $P[X(t)|x_0]$. These two probability functionals are related by the Jacobian $|\frac{\partial\xi}{\partial x}|$. Thus, we can as well write [12]

$$P\big[X(t)|x_0\big] \propto \exp\left[-\frac{1}{2}\int_0^\tau \xi^2(t)\,dt\right], \tag{5}$$

where the proportionality constant is different from that in Eq. (4). In Eq. (5), we then substitute the expression for $\xi(t)$ from the Langevin equation (Eq. (2)):

$$P\big[X(t)|x_0\big] \propto \exp\left[-\frac{1}{4}\int_0^\tau dt\,\frac{(m\dot{v} + U'(x,t) + \gamma(x)v)^2}{\gamma(x)T}\right]. \tag{6}$$

For the reverse process, $v \to -v$, but the Jacobian is same. The ratio of probability of the forward to the reverse path can be readily shown to be [12,24]

$$\begin{aligned}\frac{P[X(t)|x_0]}{\tilde{P}[\tilde{X}(t)|\tilde{x}_\tau]} &= \frac{\exp[-\int_0^\tau dt\,(m\dot{v} + U'(x,t) + \gamma(x)v)^2/4\gamma(x)T]}{\exp[-\int_0^\tau dt\,(m\dot{v} + U'(x,t) - \gamma(x)v)^2/4\gamma(x)T]} \\ &= \exp\left[-\int_0^\tau dt\,\frac{4m\gamma(x)\dot{v}v + 4U'(x,t)\gamma(x)v}{4\gamma(x)T}\right] \\ &= \exp\left[-\beta\int_0^\tau dt\,\big(m\dot{v}v + U'(x,t)v\big)\right] \\ &= e^{\beta Q},\end{aligned} \tag{7}$$

where Q is the heat dissipated by the system into the bath, defined as

$$\begin{aligned}Q &\equiv \int_0^\tau \big\{\gamma(x)v - \sqrt{2\gamma(x)T}\xi(t)\big\}v\,dt \\ &= -\int_0^\tau \big\{m\dot{v} + U'(x,t)\big\}v\,dt.\end{aligned} \tag{8}$$

This definition follow from the stochastic energetics developed by Sekimoto [25,26] from the definition of first law using Langevin dynamics. Eq. (7) is the celebrated CFT, from which several FT follow.

2.2. Integral and detailed fluctuation theorems

We have,

$$\frac{P[X(t)|x_0]}{\tilde{P}[\tilde{X}(t)|\tilde{x}_\tau]} = e^{\beta Q}, \tag{9}$$

where Q is the heat dissipated, as obtained from the first law. Multiplying by the ratio of the initial equilibrium distributions, for forward and reverse processes, namely by $p_0(x_0)/p_1(x_\tau)$, we get [15]

$$\begin{aligned}\frac{P[X(t)|x_0]p_0(x_0)}{\tilde{P}[\tilde{X}(t)|\tilde{x}_\tau]p_1(x_\tau)} &= \frac{P[X]}{\tilde{P}[\tilde{X}]} = e^{\beta Q}\cdot\frac{e^{-\beta E_0}}{Z(\lambda_0)}\cdot\frac{Z(\lambda_\tau)}{e^{-\beta E_\tau}} \\ &= e^{\beta(Q+\Delta E-\Delta F)} = e^{\beta(W-\Delta F)}.\end{aligned} \tag{10}$$

We have used the expression for equilibrium initial distribution $p_0(x_0) = \frac{e^{-\beta E_0}}{Z(\lambda_0)}$ and $p_1(x_\tau) = \frac{e^{-\beta E_\tau}}{Z(\lambda_\tau)}$. Here, $\Delta E \equiv E_\tau - E_0$, and we have made use of the relation $Z = e^{-\beta F}$, between the partition function and the free energy. $Z(\lambda_0)$ and $Z(\lambda_\tau)$ are the partition functions corresponding to the protocol values at the initial time and the final time, respectively. In the final step, the first law for the work done on the system, $W = Q + \Delta E$, has been invoked. The above relation can be readily converted to the Crooks work theorem [16], given by