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LETTER TO THE EDITOR

Fluctuation theorem in rachet system

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Abstract

The fluctuation theorem (FT) has been studied as a far from equilibrium theorem, which relates the symmetry of entropy production. To investigate the application of this theorem, especially to biological physics, we consider the FT for a tilted rachet system. Under natural assumptions, the FT for steady state is derived.

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1. Introduction

Since the discovery by Evans *et al* [1], the fluctuation theorem (FT) has been studied in many situations, both stochastic [2–4] and deterministic [1, 5]; though systems and interpretations differ, the FT has a universal form:

$$\frac{\operatorname{Prob}(\Delta S = A)}{\operatorname{Prob}(\Delta S = -A)} \simeq e^{\Delta S} \tag{1}$$

where ΔS is the entropy generated, and Prob($\Delta S = A$) is the probability for $\Delta S = A$. It is interesting that a FT type of relation universally holds, but its direct experimental application is not known. (Though Jarzynski's equality [6] is closely related to FT and has been used in the experiment, this equality is not the FT itself; in this sense application of Jarzynski's equality is not direct.) So, we would like to derive the FT for a rachet system, because it relates biological physics, and direct application of the FT is expected. The analysis is based on the Langevin treatment. Kurchan showed that for a Langevin system, if the initial state is Gibbsian, the FT holds generally [3]. Though we consider the Langevin treatment, the result does not depend on the initial condition and in this sense our interest is different from that of Kurchan.

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2. Rachet system

In this paper we consider the rachet system, namely a particle on a periodic potential V(x + L) = V(x) is dragged by a constant load force *F*. Then, the effective potential the particle feels is $V_{\text{eff}} \equiv V(x) - xF$. If the potential barrier is high enough, the particle could be considered to be almost at equilibrium and might satisfy the detailed balance relation. Indeed, the quantitative argument is given in the review by Reimann [7]. We summarize the work by Reimann.

We consider a system that a particle on a periodic potential (period L) is dragged by a constant load force F. The motion of this particle can be described by the Langevin equation

$$\eta \frac{\mathrm{d}}{\mathrm{d}t} x(t) = -\frac{\mathrm{d}}{\mathrm{d}x} V_{\mathrm{eff}}(x) + \xi(t)$$
$$V_{\mathrm{eff}}(x) \equiv V(x) - Fx$$
$$\langle \xi(t)\xi(s) \rangle = \sqrt{2\eta k_B T} \delta(t-s).$$

The corresponding Fokker–Planck equation becomes

$$\frac{\partial}{\partial t}P(x,t) = \frac{\partial}{\partial x}\left(\frac{\mathrm{d}V_{\mathrm{eff}}}{\mathrm{d}x}\frac{1}{\eta} + \frac{k_BT}{\eta}\frac{\partial}{\partial x}\right)P(x,t) = -\frac{\partial}{\partial x}J(x,t).$$
(2)

Here J(x, t) is the probability current. Then at a steady state, the reduced probability current

$$\hat{J}(x,t) \equiv \sum_{n=-\infty}^{\infty} J(x+nL,t)$$
(3)

becomes

$$\hat{J}^{\text{st}} = N\left(1 - \exp\left(-\frac{FL}{k_B T}\right)\right)$$

$$N = \frac{k_B T}{\eta} \left(\int_0^L dx \int_x^{x+L} dy \exp\left(\frac{V_{\text{eff}}(y) - V_{\text{eff}}(x)}{k_B T}\right)\right)^{-1}.$$
(4)

If in each period *L* there exists one minimum x_{\min} and one maximum x_{\max} , and the system is in the weak noise regime $k_BT \ll \Delta V_{\text{eff}} \equiv V_{\text{eff}}(x_{\max}) - V_{\text{eff}}(x_{\min})$, the saddle-point approximation gives the following probability current:

$$\hat{J}^{\text{st}} = k_{+} - k_{-}$$

$$k_{+} = \frac{\left|\frac{d^{2}}{dx^{2}}V_{\text{eff}}(x_{\text{max}})\frac{d^{2}}{dx^{2}}V_{\text{eff}}(x_{\text{min}})\right|^{\frac{1}{2}}}{2\pi\eta}\exp\left(-\frac{\Delta V_{\text{eff}}}{k_{B}T}\right)$$

$$k_{-} = k_{+}\exp\left(-\frac{FL}{k_{B}T}\right).$$
(5)

Here k_+ and k_- are the Kramers escape rates, the probabilities per unit time for a particle near a potential minimum to escape to the right minimum and left minimum respectively (figure 1). These k_+ and k_- satisfy the detailed balance relation

$$\frac{k_+}{k_-} = \exp\left(\frac{FL}{k_BT}\right). \tag{6}$$

TiltedRachet

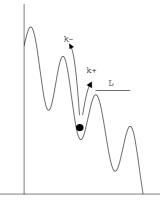


Figure 1. A particle hopping on a tilted potential.

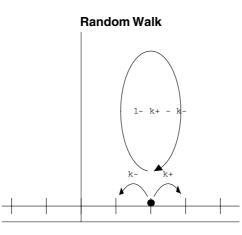


Figure 2. Biased random walk of a particle.

3. Derivation of steady-state fluctuation theorem

Because of the assumption $k_B T \ll \Delta V_{\text{eff}}$, we can describe the motion of a particle in terms of a biased random walk. Namely, it is sufficient to observe only the local minimum of effective potential and on which minimum the particle (approximately) exists at each discrete time $t = 0, \tau, 2\tau, \ldots$. It is natural to assume that a particle hops only to the nearest-neighbour local minima: to the right minimum with probability k_+ , to the left minimum with k_- , and it does not move with probability $1 - (k_+ + k_-)$.

Then the motion of a particle follows the biased random walk. A particle hops to right, left and remains with probabilities k_+ , k_- and $1 - (k_+ + k_-)$, respectively (figure 2). Next we consider the probability $\pi_n(k)$ which is the probability that after *n* unit time, a particle moves *k* towards the right. Here we can show the equation

$$\frac{\pi_n(k)}{\pi_n(-k)} = \left(\frac{k_+}{k_-}\right)^k.$$
(7)

One can prove this equation via following one-to-one correspondence: consider any process that causes the movement k after n unit time. The process is constituted by movements: k + l

times towards the right, *l* times towards the left and n - k - 2l times remaining. This process occurs with the probability

$$\frac{n!}{(k+l)!l!(n-k-2l)!}k_{+}^{k+l}k_{-}^{l}(1-k_{+}-k_{-})^{n-k-2l}.$$
(8)

The corresponding opposite process: *l* times towards the right, k + l times towards the left and n - k - 2l times remaining, occurs with the probability

$$\frac{n!}{(k+l)!l!(n-k-2l)!}k_{+}^{l}k_{-}^{k+l}(1-k_{+}-k_{-})^{n-k-2l}.$$
(9)

So the ratio of the probabilities that these two opposite processes occur is $\left(\frac{k_+}{k_-}\right)^k$. This is valid for any *l*, and the equation is derived.

Then we substitute the detailed balance relation for Kramers escape rate $\frac{k_+}{k_-} = \exp(\frac{FL}{k_BT})$ into the above equation, and obtain the following expression:

$$\frac{\pi_n(k)}{\pi_n(-k)} = \exp\left(\frac{FLk}{k_BT}\right).$$
(10)

We define the entropy generated $\Delta S \equiv \frac{\Delta Q}{k_B T}$, where $\Delta Q = FLk$ is the Joule heat. ΔS can be considered as the entropy generated, since the work done on the system externally will be entirely dissipated, and there is no contribution to the internal energy. Finally, we take the continuous limit, $n \to t$, $Lk \to x$, and obtain the steady-state fluctuation theorem

$$\frac{\pi_t(\Delta S)}{\pi_t(-\Delta S)} = e^{\Delta S}.$$
(11)

4. Discussion

The FT for a rachet system is derived. The FT derived here is applicable to any system which obeys a biased random walk and satisfies the detailed balance relation.

Especially, a complete example was recently given by Nishiyama *et al* [8]. They performed an experiment where a single kinesin externally forced moves along a microtubule obeying a biased random walk with regular 8 nm steps. And they measured the ratio of the forward to backward movements at each load force 1–9 pN, the result agrees well with the detailed balance relation. The FT derived in this letter would therefore be valid for this system.

Because the derivation of the FT consists of two parts, identity (6) and detailed balance relation, there is the possibility that under some condition detailed balance does not hold and the FT should be modified. This modification of the FT is an open problem.

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