Calculation of Correlation Functions in Terms of Fluctuation Relation

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Abstract

We derive a relation similar to the fluctuation theorem for work done on a system obeying Langevin dynamics with thermal and colored noises. Then, we propose a method of calculating the correlation function of the colored noise by using this fluctuation relation.

Key words: fluctuation theorem, correlation function of colored noise, Langevin dynamics

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1 Introduction

Fluctuation theorems (FT) [1] have been studied as one of exact relations valid in far from equilibrium regime. They state the symmetry of fluctuation of entropy production $\Delta S$: 

$$\left( \lim_{t \to \infty} \right) \frac{\pi_t(\Delta S = A)}{\pi_t(\Delta S = -A)} = A,$$  

where $\pi_t(\Delta S = A)$ denotes the probability density that a system’s entropy production during time interval $t$ equals to $A$, and the limit of $t \to +\infty$ is taken or not depending on systems. Although interpretations and systems differ, this expression universally holds [7,8,9,10,11,12].

Jarzynski equality [2] was shown to be derived from FT [3] and was applied, e.g. to evaluate the free energy of biological systems [4]. It is even more inter-

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testing to investigate direct applications of FT. In this letter, we der ivi
derive a FT-like relation (FR) for work done on a system obeying Langevin
dynamics. In addition to the thermal noise, a colored noise is assumed to be applied. Then,
this FR is shown to be used to evaluate a correlation function of the colored
noise from the fluctuations of the work done. Such correlation functions would
provide information about driving force in nonequilibrium regime and we ex-
pect that the FR-aided analysis is useful to investigate the behaviors of single
molecular motors [5] or micro/nano machines.

2 Fluctuation Relation and Correlation Function

We consider a system described by a Langevin equation:

\[ \int_{-\infty}^{t} \Gamma(t-t')v(t')dt' = f + \xi(t) + \Xi(t) \]  \( (2) \)

\[ \langle \xi(t)\xi(t') \rangle = \frac{1}{\beta} \Gamma(t-t') \]  \( (3) \)

\[ \langle \Xi(t)\Xi(t') \rangle = M(t-t') \]  \( (4) \)

\[ \langle \xi(t) \rangle = \langle \Xi(t) \rangle = 0 , \]  \( (5) \)

where \( \xi(t) \) and \( \Xi(t) \) are the thermal and colored noises, respectively, \( f \) stands
for a constant external force, and \( \beta \) is the inverse temperature. The noises \( \xi(t) \)
and \( \Xi(t) \) are assumed to be Gaussian and independent from each other. Eq.(3)
is nothing but the fluctuation dissipation relation. We assume that the memory
kernel \( \Gamma(t) \) exponentially decays as \( \Gamma(t) = \Gamma_0 e^{-\gamma t} \). Such a Langevin equation
would provide a phenomenological description of the motion of molecular mo-
tors as pointed out by Harada [6], where the energy balance in the molecular
motor was investigated.

Now, we introduce the work \( \Sigma_t \) done on the system by the external force \( f \)
during the time interval \( t \):

\[ \Sigma_t \equiv \beta \int_{0}^{t} ds f v(s) \]  \( (6) \)

We denote the probability density of \( \Sigma_t \) being \( A \) as \( \pi_t(\Sigma_t = A) \). As we shall
show later, one then obtains a fluctuation relation (FR):

\[ F(t) \equiv t \left( \frac{1}{A} \log \frac{\pi_t(\Sigma_t = A)}{\pi_t(\Sigma_t = -A)} \right)^{-1} - 1 \]
\[
\beta \int_0^t ds \int_0^{s'} \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega (\gamma^2 + \Gamma_0^2) \hat{M}(\omega)e^{i\omega(s-s')} ,
\]  
(7)

where \( \hat{M}(\omega) \) is the Fourier transformation of the correlation function \( M(t) \) of the colored noise. Note that this FR is different from usual FT's, because it says nothing about entropy production, but only refers to the work done by an external force.

The FR (7) leads to a differential equation of \( M(t) \):

\[
-\frac{d^2}{dt^2}M(t) + \gamma^2 M(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega (\gamma^2 + \Gamma_0^2) \hat{M}(\omega)e^{i\omega t} = \frac{\gamma \Gamma_0}{\beta} \frac{d^2}{dt^2}F(t) .
\]  
(8)

The quantity \( F(t) \) defined in (7) can be measured experimentally by observing individual trajectories and, thus, one can determine \( M(t) \) provided two parameters \( \gamma \) and \( \Gamma_0 \) are known. We note that \( F(t) \) is independent of \( A \).

So far we have assumed \( \langle \Xi(t) \rangle = 0 \) for simplicity. However, the case of \( \langle \Xi(t) \rangle \equiv \Xi_0 \neq 0 \) can be treated in the same way and one can show that the function

\[
\tilde{F}(t) \equiv t \left\{ \frac{1}{A} \log \frac{\pi t (\Sigma_t = A)}{\pi t (\Sigma_t = -A)} \right\}^{-1} - \frac{f}{f + \langle \Xi_0 \rangle}
\]

instead of \( F(t) \) satisfies

\[
-\frac{d^2}{dt^2}M(t) + \gamma^2 M(t) = \frac{\gamma (f + \Xi_0) \Gamma_0}{\beta f} \frac{d^2}{dt^2}\tilde{F}(t) .
\]  
(9)

In this case again, the correlation function \( M(t) \) of the colored noise can be evaluated experimentally.

### 3 Derivation of Fluctuation Relation

In this section, we shall derive (7). Because \( \Sigma_t \) is a Gaussian process, in order to determine \( \pi_t(\Sigma_t = A) \), it is sufficient to calculate the mean value \( \langle \Sigma_t \rangle \), and the variance \( \langle \Sigma_t^2 \rangle - \langle \Sigma_t \rangle^2 \).

With the aid of the Fourier transformation, one obtains following expression :

\[
v(t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \hat{f}(\omega) + \hat{\xi}(\omega) + \hat{\Xi}(\omega) \frac{e^{i\omega t}}{\Gamma(\omega)},
\]  
(10)
where \( \hat{\Gamma}(\omega) \equiv \frac{\Gamma_\omega}{\gamma + i\omega} \) is the Fourier-Laplace transformation of \( \Gamma(t) \), and \( \hat{f}(\omega) \equiv 2\pi f \delta(\omega) \), \( \hat{\xi}(\omega) \) and \( \hat{\Xi}(\omega) \) are the Fourier transformations of \( f, \xi(t) \), and \( \Xi(t) \), respectively. Therefore, (5) leads to

\[
\langle \Sigma_t \rangle = \beta f^2 \frac{\gamma}{\Gamma_0} t
\]

From \( \langle \hat{\Xi}(\omega)\hat{\Xi}(\omega') \rangle = 2\pi \hat{M}(\omega) \delta(\omega+\omega') \) and the fluctuation dissipation theorem: \( \langle \hat{\xi}(\omega)\hat{\xi}(\omega') \rangle = \frac{4\pi \Re \hat{\Gamma}(\omega) \delta(\omega+\omega')}{\beta} \), we obtain the variance of \( \Sigma_t \):

\[
\langle \Sigma_t^2 \rangle - \langle \Sigma_t \rangle^2 = \beta \frac{2\gamma f^2}{\Gamma_0} t
+ \beta^2 f^2 \int_0^t ds \int_0^t ds' \left( \frac{1}{2\pi} \right)^2 \int_{-\infty}^{\infty} d\omega \int_{-\infty}^{\infty} d\omega' \frac{\langle \hat{\Xi}(\omega)\hat{\Xi}(\omega') \rangle}{\Gamma(\omega)\Gamma(\omega')} e^{i\omega s} e^{i\omega' s'}
\]

\[
= \beta \frac{2\gamma f^2}{\Gamma_0} t + \beta^2 f^2 \int_0^t ds \int_0^t ds' \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \frac{\omega^2 + \omega^2}{\Gamma_0} \hat{M}(\omega) e^{i\omega(s-s')}.
\]

Substituting the mean value \( \langle \Sigma_t \rangle \) and the variance \( \langle \Sigma_t^2 \rangle - \langle \Sigma_t \rangle^2 \) into

\[
\log \frac{\pi t (\Sigma_t = A)}{\pi t (\Sigma_t = -A)} = \frac{2\langle \Sigma_t \rangle A}{\langle \Sigma_t^2 \rangle - \langle \Sigma_t \rangle^2},
\]

one obtains the fluctuation relation for work done by an external force: (7).

To summarize, we derived a fluctuation relation for the work done on the system: eqs.(7) and (8). Eq.(7) has a form of the fluctuation theorem with modification due to \( \langle \Xi(t)\Xi(t') \rangle \). An important point is that the right hand side of (8) is measurable experimentally, and thus, we can evaluate the correlation function \( \langle \Xi(t)\Xi(t') \rangle \) of the nonthermal colored noise.

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