Variational formula for experimental determination of high-order correlations of current fluctuations in driven systems

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For Brownian motion of a single particle subject to a tilted periodic potential on a ring, we propose a formula for experimentally determining the cumulant generating function of time-averaged current without measurements of current fluctuations. We first derive this formula phenomenologically on the basis of two key relations: a fluctuation relation associated with Onsager’s principle of the least energy dissipation in a sufficiently local region and an additivity relation by which spatially inhomogeneous fluctuations can be properly considered. We then derive the formula without any phenomenological assumptions. We also demonstrate its practical advantage by numerical experiments.

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Introduction: Transportation properties in linear response regime out of equilibrium are determined by the second-order correlation of time-averaged current fluctuation in equilibrium [1]. As an extension of this well-established formula, a nonlinear response formula was derived [2], where stronger non-linearity arises when the third and higher order correlations are more relevant. Thus, toward a systematic understanding of strongly nonlinear transportation, a universal law concerning high-order correlations must be considered.

In general, let $\dot{I}$ be a time-averaged current during a time interval $\tau$. Its statistical property is characterized by a cumulant generating function $G(h)$, which is defined by

$$e^{\tau G(h)} = \langle e^{\tau \dot{I}} \rangle$$

for sufficiently large $\tau$. In recent years, $G(h)$ has been studied theoretically for several models [3-10], partly motivated by its symmetry property called fluctuation theorem [11]. However, it is difficult to experimentally measure $G(h)$ when the distribution of $\dot{I}$ deviates far from the Gaussian. Since physically important quantities should be obtained experimentally, there should be a formula for making $G(h)$ measurable.

Here, let us recall Einstein’s theory for macroscopic fluctuation of thermodynamic variables in equilibrium. As an example, the cumulant generating function of space-averaged magnetization $\hat{m}$ in magnetic materials without a magnetic field is equivalent to the Gibbs free energy density as a function of the magnetic field, and the thermodynamic functions can be determined by measurements of heat capacity and susceptibility for any magnetic field and temperature. This implies that the cumulant generating function of $\hat{m}$ is obtained without measurements of fluctuations. A universal idea behind Einstein’s theory is that when a state is determined by an extreme condition of a function, fluctuation properties at more microscopic scales are described by the variational function. The relation between the least action principle in classical mechanics and the path-integral formulation of quantum mechanics follows the same idea. We thus conjecture that the cumulant generating function $G(h)$ of $\dot{I}$ might be identified with a variational function associated with a variational principle that determines a steady state.

In this Letter, we study Brownian motion of a single particle subject to a tilted periodic potential on a ring. Starting from the analysis of a simple example based on the least energy dissipation principle [1], we propose a phenomenological formula for experimentally determining the cumulant generating function of time-averaged current. We then derive the formula theoretically and measure $G(h)$ in numerical experiments.

Basic idea: We investigate an electric circuit where three resistances, $R_0$, $R_1$ and $R_2$, are connected in series under voltage $V_0$. In particular, in the limiting case that $V_0 \to \infty$ and $R_0 \to \infty$ with $I = V_0/R_0$ fixed, the system is assumed to be in the constant-current environment. Furthermore, we can impose the constraint that the voltages over the resistance $R_1$ and $R_2$ are fixed as $V_1$ and $V_2$, respectively. The total energy dissipation ratio in this system is given by

$$\Phi(V_1, V_2|I) = \frac{V_1^2}{R_1} + \frac{V_2^2}{R_2} - 2(V_1 + V_2)I,$$

where we ignore a contribution independent of $V_1$ and $V_2$. When we remove the voltage constraint, the values of $V_1$ and $V_2$ are determined by the condition that the current is equal to $I$. Here, these values minimize $\Phi(V_1, V_2|I)$. This is an example of the least energy dissipation principle.

We next investigate another electric circuit, where two resistances, $R_1$ and $R_2$, are connected in series and the resistance $R_0$ is connected in a parallel way under the total current $I_0$. In the limiting case that $I_0 \to \infty$ and $R_0 \to 0$ with $V = R_0I_0$ fixed, the system is assumed to be in the constant-voltage environment. We can impose the constraint that the current passing the resistances $R_1$
and \( R_2 \) is fixed as \( I \). The total energy dissipation ratio in this system is given by

\[
\Psi(I|V) = (R_1 + R_2)I^2 - 2VI,
\]

(3)

where we ignore a contribution independent of \( I \). Without the current constraint, the value of \( I \) is determined by the condition that the voltage is equal to \( V \). Here, this value minimizes \( \Psi(I|V) \). This is another example of the least energy dissipation principle.

Now, a variational principle is expected to be related to the description of fluctuation properties as discussed in Introduction. For example, the probability of time-averaged current fluctuations in the constant-voltage environment is given as

\[
\text{Prob}(I|V) \approx e^{-\tau \Phi(\Psi(I|V) + c_0)}.
\]

(4)

where \( c_0 \) is the normalization constant and the coefficient \( 4T \) respects the fluctuation-dissipation relation and the Boltzmann constant is set to unity. Then, the cumulant generating function \( G(h|V) \) is determined by

\[
G(h|V) = -\frac{1}{4T} \min_I [\Phi(\Psi(I|V) - 4ThI + c_0)].
\]

(5)

The condition \( G(h = 0|V) = 0 \) gives \( c_0 = -\Psi(I|V) \), where \( I_s \) represents the steady current. Although \( \Phi(\cdot) \) is a simple mathematical expression, we here attempt to rewrite it so as to be measured experimentally. The idea is to consider a modified system in which an extra voltage \( v \) in addition to \( V \) is applied. We define \( v_{i,s} \equiv vR_i/(R_1 + R_2) \) which represents the allocation of the extra voltage \( v \) in the circuit. We also denote \( I_{i,s} \) the steady current for the modified system. By using these quantities, we can express \( \Psi(I|V) - 4ThI + c_0 \) as

\[
\Phi(v_{1,s}, v_{2,s}|I_{i,s}) + \sum_{i=1}^{2} R_i(I - I_{i,s})^2 - 2I(2Th - v).
\]

(6)

By choosing \( v = 2Th \) and minimizing \( \Phi(\cdot) \) in terms of \( I \), we obtain \( G(h|V) = -\Phi(v_{1,s}, v_{2,s}|I_{i,s})/(4T) \). The variational principle in the first example leads us to rewrite it as an additive form

\[
G(h|V) = -\frac{1}{4T} \min_{v_{1,s} + v_{2,s} = 2Th} \sum_{i=1}^{2} \left[ \frac{v_i^2}{R_i} - 2I_{i,s}v_i \right].
\]

(7)

This additivity relation is the basic formula which we extend so as to apply more general cases. Since the voltages can be controlled experimentally, the right-hand side of \( \Phi(\cdot) \) is obtained experimentally. Although the formula is derived for the simple system, the result is quite suggestive. The assumption for the formula is that the least energy dissipation principle and the fluctuation-dissipation relation hold locally in space. Although this assumption is not always valid, many non-equilibrium systems are included in this class. Below we apply the relation \( \Phi(\cdot) \) to the Brownian motion out of equilibrium.

**Main Result:** The system we study consists of a single Brownian particle on a ring with a size of \( L \). Its motion is described by a Langevin equation

\[
\gamma \dot{x} = f - \frac{\partial U}{\partial x} + \xi,
\]

(8)

where \( \dot{x} \equiv dx/dt \) and \( \xi \) is the noise satisfying \( \langle \xi(t)\xi(t') \rangle = 2T \gamma \delta(t - t') \). \( \gamma \) represents a friction constant, \( f \) a uniform driving force, and \( U(x) \) a periodic potential. The external force acting on the particle is written as \( F(x) = f - \partial U(x)/\partial x \). It should be noted that the Langevin equation \( \gamma \delta(t - t') \) corresponds to experimental systems that have been studied with the aim of testing new ideas in non-equilibrium statistical mechanics \[12–14\]. We are particularly concerned with the cumulant generating function \( G(h) \) defined in \( \Phi(\cdot) \) with \( I \) replaced by

\[
\dot{v} = \frac{1}{T} \int_0^t dt \frac{dx}{dt}.
\]

(9)

Throughout this letter, the boldface font is used to indicate a function of \( x \).

Here, in order to find a formula similar to \( \Phi(\cdot) \), we apply an extra force \( u(x) \) in addition to \( F(x) \) with an interpretation that \( F(x) \Delta x \) and \( u(x) \Delta x \) correspond to the voltage and the excess voltage over the interval \( [x, x + \Delta x] \), respectively. We consider an empirical probability density \( \rho(x) \) and its current \( j(x) \) obtained by measurement during a finite time interval \( \tau \). That is, \( \rho(x) \equiv \int_0^\tau dt \delta(x - x(t))/\tau \) and \( j(x) \equiv \int_0^\tau dt \delta(x - x(t) - \dot{x})/\tau \), where \( \delta(x) \) is the Stratonovich rule of the multiplication. In the limit \( \tau \to \infty \), \( j(x) \to J_s^u \) and \( \rho(x) \to \rho_s^u(x) \), where the steady probability density \( \rho_s^u(x) \) and the spatially homogeneous current \( J_s^u \) for this modified system with the extra force \( u \) are determined by

\[
J_s^u = \frac{1}{\gamma} \rho_s^u(F + u) - \frac{T}{\gamma} \frac{\partial}{\partial x} \rho_s^u.
\]

(10)

This shows that the resistance in the interval \( [x, x + \Delta x] \) corresponds to \( \gamma(\Delta x)/\rho_s^u(x) \). Finally, since the current \( I \) corresponds to \( \int_0^L dx j(x)/L = \dot{v}/L \), \( h \) in the formula for the time averaged current is replaced by \( hL \) for the case of cumulant generating function \( G(h) \) for \( \dot{v} \). That is, the constraint condition \( v_1 + v_2 = 2Th \) becomes

\[
\int_0^L dx u(x) = 2ThL.
\]

(11)

From these correspondences, we heuristically derive

\[
G(h) = -\frac{1}{4T} \min_{u: \int_0^L dx u(x) = 2ThL} \mathcal{G}(u),
\]

(12)

with

\[
\mathcal{G}(u) = \int_0^L dx \left[ \frac{\rho_s^u(x)}{\gamma} u(x)^2 - 2J_s^u u(x) \right].
\]

(13)
That is, $G(h)$ is proportional to the minimum energy dissipation of the extra force $u(x)$ when the system is assumed to be in constant-current environment of the current $J^x$ with $J^L dxu(x) = 2ThL$. The formula (12) with (13) is the main claim of this Letter.

We determine the optimal force $u_{\text{opt}}(x)$ that satisfies $\delta G = G(u + \delta u) - G(u)$ with the condition (11). By calculating $\delta G \equiv G(u + \delta u) - G(u)$ explicitly, we find that $\delta G = 0$ leads to

$$K = \frac{1}{\gamma} \left( F + \frac{u_{\text{opt}}}{2} \right) u_{\text{opt}} + \frac{T}{\gamma} \partial_x u_{\text{opt}},$$

(14)

where $K$ is a constant. Differentiating the both-sides with respect to $x$, we obtain $u_{\text{opt}}(x)$ under the periodic boundary condition. The substitution of the obtained result $u_{\text{opt}}$ into (14) leads to $K$. This constant $K$ is significant. Indeed, by multiplying $p_{\text{opt}}^u$ to (14) and $u_{\text{opt}}$ to (11) and by considering the difference between them, we obtain $K = 2TG(h)$. Furthermore, for the non-linear differential equation (14) with $K = 2TG(h)$, we perform a Cole-Hopf transformation defined by $u_{\text{opt}}(x) = 2T(h + \partial \log \psi(x))$, where $\psi(x) > 0$. We then derive a linear eigenvalue equation $L_h \psi = G(h) \psi$, where the operator $L_h$ is defined by

$$L_h \psi \equiv \frac{F}{\gamma} \partial_x \psi + \frac{T}{\gamma} \partial_x^2 \psi \cdot$$

(15)

From the positivity of $\psi$, $G(h)$ turns out to be equal to the maximum eigenvalue $\lambda_{\text{max}}$ of the operator $L_h$ and $u_{\text{opt}}$ is related to the corresponding eigenfunction. Examples of $G(h)$ thus determined uniquely are displayed in the left-side of Fig. 1.

Now, we prove (12) without employing any phenomenological assumptions. For a stochastic variable $y(t) \equiv \int_{0}^{t} dx \phi(x)$, we denote by $P(y,t)$ the probability density that the value $y$ takes at time $t$. We then have $\exp(\sigma G(h)) = \int dy P(y,t) \exp(hy)$. Here, the function $Q(y,t) \equiv P(y,t) \exp(hy)$ obeys $\partial_t Q = \mathcal{M}_h \rho$, where

$$\mathcal{M}_h \rho \equiv \frac{1}{\gamma} (\partial_y - h) (F(y) \cdot \rho) + \frac{T}{\gamma} \partial_y \rho \cdot$$

(16)

We denote the maximum eigenvalue of the operator $\mathcal{M}_h$ by $\mu_{\text{max}}$. Since $Q(y,t) \simeq e^{\mu_{\text{max}} t}$ for sufficiently large $t$, $G(h)$ is equal to $\mu_{\text{max}}$. (See a related result in Ref. 1.) By comparing (15) and (16), we find $L_h \psi = \mu_{\text{max}} \psi$. Thus, $\lambda_{\text{max}} = \mu_{\text{max}}$. Since the eigenvalue equation $L_h \psi = G(h) \psi$ is equivalent to the variational form (12) with (13), we end the proof. This method of derivation of the formula can also be applied to Langevin equations in any dimensions. See Ref. 12 for details.

The formula (12) is closely related to the so-called additivity principle of $\langle x(t) \rangle_{0 \leq t \leq \tau}$. We mention the relation explicitly. Let us consider the probability density of $J = \tilde{v}/L$, which is expected to possess a large deviation property

$$\text{Prob}(\tilde{J} = J) \simeq e^{-\tau \Gamma(J)}.$$

(17)

Through mapping from (8) to fluctuating hydrodynamics (16), we can apply the additivity principle to the continuous description of the fluctuating density field. The result is

$$\Gamma(J) = \min_{\rho} \int_{0}^{L} dx \frac{(J - J^x(x; \rho))^2}{4T \rho(x)/\gamma},$$

(18)

where $J^x(x; \rho) \equiv \rho(F(x) + u(x))/\gamma - TO_{\text{opt}} / \gamma$ for any $u(x)$. Since $G(h)$ is connected to $\Gamma(J)$ as $G(h) = \max_{J} [hLJ - \Gamma(J)]$, we obtain

$$G(h) = -\frac{1}{4T} \min_{J, \rho} \int_{0}^{L} dx \phi(x; J, \rho),$$

(19)

where

$$\phi(x) = \frac{\rho(x)}{\gamma} u(x)^2 - 2u(x)j^x_n(x; \rho) + \frac{\gamma}{\rho(x)} [J - j^x_n(x; \rho)]^2.$$

(20)

under the constraint condition (11). We make a variable transformation from $\rho$ to $u$ by $\partial_x j^x_n(x; \rho) = 0$. Explicitly, for a given $u$, we can determine $J^x_n$ and $\rho^u_n$ uniquely as $j^x_n(x; \rho^u_n) = J^x_n$. The minimization with respect to $J$ in (19) is achieved by $J = J^x_n$, and $\int_{0}^{L} dx \phi(x; J, \rho^u_n)$ becomes $G(u)$. Thus, (19) leads to the formula (12).

**Experiment:** We consider the experimental measurement of $G(h)$. In the standard method, $G(h)$ may be determined from the measurements of cumulants. However, high-order cumulants are quite difficult to be measured experimentally. Here, we claim that our formula can provide $G(h)$ experimentally if we can control the external force and know the value of the temperature $T$ and the friction constant $\gamma$. The method is as follows.

We measure a trajectory $(x(t))_{0 \leq t \leq \tau}$ for the system with an extra force $w(x)$. From this data, we define

$$\hat{G}_\tau(w) \equiv \frac{1}{\tau} \int_{0}^{\tau} dt \left[ \frac{w(x(t))^2}{\gamma} - 2\dot{x}(t) \circ w(x(t)) \right].$$

(21)

Note that $\hat{G}_\tau(w) \rightarrow G(w)$ in the limit $\tau \rightarrow \infty$. Thus, if we know the optimal force $u_{\text{opt}}$, the approximate value of $G(h)$ is obtained from $\hat{G}_\tau(w)$ by setting $w = u_{\text{opt}}$. Here, we have an identity

$$G(u_{\text{opt}}) = -4ThJ^w - \int_{0}^{L} dx \frac{\rho^w_{\text{opt}}}{\gamma} u_{\text{opt}}(u_{\text{opt}} - 2w)$$

(22)

for any $w$, which can be derived from the calculation of $G(u_{\text{opt}}) - G(w)$ with the aid of (10) and (11). We express $u_{\text{opt}}(x) = 2Th + \sum_{n=-N}^{N} \phi_n(x)$, where $\phi_n(x) = \cos(2\pi nx/L)$ for $n \geq 0$, $\phi_n(x) = \sin(2\pi nx/L)$ for $n < 0$, $a_0 = 0$, and $N$ is the truncation number of the approximation of the force $u_{\text{opt}}(x)$. Since (21) holds for any $w$, we determine $(a_n)_{n=-N}^{N}$ by preparing $2N + 1$ forces $w^{(i)}(x)$, $N \leq i \leq N$. Concretely, by using the trajectory $x^{(i)}(t)$ for each $w^{(i)}(x) = 5T\phi_i(x)/L$, the right-hand side of (21) is approximated as

$$\hat{H}_\tau(w^{(i)}) \equiv \frac{1}{\tau} \int_{0}^{\tau} dt \hat{H}^{(i)}(t),$$

(22)
where
\[ \mathcal{H}^{(i)}(t) = -4T \dot{x}^{(i)}(t) + 2 \sum \phi_n(x^{(i)}(t)) \dot{w}^{(i)}(x^{(i)}(t)) a_n \]
\[ - \frac{1}{2} \sum \phi_n(x^{(i)}(t)) \phi_m(x^{(i)}(t)) a_n a_m. \]  

(23)

Since \( \tilde{H}_\infty(w^{(i)}) \) is independent of \( w^{(i)} \), we consider the following equation for \( (a_n)^N_{n=-N} \):
\[ \tilde{H}_r(w^{(i)}) = \tilde{H}_r(w^{(i)}+1), \]  
(24)

where \( -N \leq i < N \). By solving (24), we obtain an approximation of \( u_{opt}(x) \). The approximation becomes more accurate for larger \( N \) and larger \( \tau \). In the right-side of Fig. 1, we display an example of the measurement of \( G(h) \) in numerical experiments.

**FIG. 1:** (color online) \( G(h) \) for the Langevin equation (6) with \( U(x) = U_0 \cos(2\pi x/L) \). Quantities are converted to dimensionless forms by setting \( \gamma = T = L = 1 \). We fix \( f = 1 \).

(Left:) Numerical calculation of \( K = 2T G(h) \) in (13) for \( U_0 = 0 \) (red solid line), 3 (green dashed line), and 5 (blue dotted line).

(Right:) Experimental measurement for the system with \( U_0 = 3 \). We assume to know \( T = \gamma = 1 \) and determined \( G(h) \) experimentally from trajectories \( (x(t)) \) according to the method described in the text. \( N = 5 \) and \( \tau = 25 \) (triangle symbols), 1000 (square symbols), and 4000 (circle symbols). The error-bars are within the symbols. The dashed line is the same as that in the left-side.

**Concluding remarks:** In this Letter, we have proposed the formula (12) for a driven Brownian motion described by (5). We have demonstrated that \( G(h) \) can be determined experimentally from \( T, \gamma \), and trajectories of the modified system with an external force. Note that the formula yields an expression of the \( k \)-th order cumulant \( C_k = \tau^{k-1} \langle \dot{v}^k \rangle \), where \( C_1 \) and \( C_2/2 \) are equal to the average velocity and diffusion constant of the Brownian particle, respectively. The result reproduces the known expression for the diffusion constant \( \left[ \right. \) in the simplest manner. Furthermore, (12) can be extended to more general bulk-driven systems when we assume fluctuating hydrodynamics. We express \( G(h) \) by a path-integral expression, and if it is determined by the contribution of a saddle configuration, the formula (12) is valid, as for the case of (8). However, there are many systems for which the condition is not satisfied, as investigated in Refs. [4, 7]. (See also sections 3 and 4 in [18] for directly related discussions on the problem in this Letter.) Future work will concern the determination of the range of the application of the formula. We believe that our theory for the derivation provides a sound approach in studying this problem. We also wish to present non-trivial predictions by employing the formulas for interacting particles systems. We hope that our formula will be studied theoretically, numerically, and experimentally, so that the novel nature of non-equilibrium fluctuation can be uncovered.

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