Stochastic Energetics for Non-Gaussian Processes

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By introducing a new stochastic integral, we investigate the energetics of classical stochastic systems driven by non-Gaussian white noises. In particular, we introduce a decomposition of the total energy difference into the work and the heat for each trajectory, and derive a formula to calculate the heat from experimental data on the dynamics. We apply our formulation and results to a Langevin system driven by a Poisson noise.

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Introduction.—Stochastic processes driven by non-Gaussian noises are shown to be powerful to analyze various natural and social phenomena: the shot noise in electrical circuits [1], Lévy flights of bumblebees [2] and human mobilities, [3] and random walks in finance and econophysics [4,5]. Moreover, non-Gaussian effects have been discussed for small thermodynamics systems such as biological molecular machines. For example, a non-Gaussian white noise has been used for modeling directed transport in Brownian motors [6,7], and the Adenosine triphosphate (ATP) reception by red blood cell membranes [8,9] has been modeled in terms of non-Gaussian noises. This Letter aims to introduce a new stochastic integral for non-Gaussian processes and apply it to small thermodynamic systems.

Recent progress in experimental technique is causing growing interest in small thermodynamic systems [10]. In such systems, thermodynamic quantities become stochastic due to environmental fluctuations that can be non-Gaussian. The thermodynamic energy balance in a single trajectory has been formulated by stochastic energetics [11] in which thermodynamic quantities, such as work and heat, are defined for each trajectory [12]. Stochastic energetics has been widely applied to theories [13–22] and experiments [23–28] of modern nonequilibrium statistical mechanics.

For Gaussian processes, it has been established that the Stratonovich-type stochastic calculus is consistent with the stochastic energetics [11]. In fact, the Stratonovich calculus has been used for experimental and numerical verifications of nonequilibrium equalities such as the fluctuation theorem [23–28]. This is because the ordinary differential calculus, such as the chain rule df/dt = (df/dx)(dx/dt), is satisfied for the Stratonovich stochastic calculus. In contrast, the Itô-type stochastic calculus needs an alternative formula, which is known as the Itô rule, instead of the ordinary chain rule. So far, however, stochastic energetics for non-Gaussian processes has not been fully investigated. It is remarkable that, as will be shown later, the Stratonovich calculus is inadequate to formulate the stochastic energetics for non-Gaussian processes.

In this Letter, we introduce a new stochastic integral, with which the ordinary differential calculus is applicable to non-Gaussian processes. Based on this, we investigate the decomposition of the total energy difference into the work and the heat for each trajectory and derive a formula that is applicable to measurements of the heat in experiments. We show that our stochastic energetics is consistent with the first law of thermodynamics.

Stochastic integrals.—Let $\hat{\xi}(t)$ be a white noise with $\langle \hat{\xi}(t) \rangle = 0$ and $\langle \hat{\xi}(t) \hat{\xi}(s) \rangle = \delta(t-s)$, where the bracket denotes the ensemble average of a stochastic variable. We consider a stochastic differential equation $d\hat{X}(t)/dt = a(\hat{X}(t)) + b(\hat{X}(t))\hat{\xi}(t)$, where $\hat{X}(t)$ is the phase-space point of a Brownian particle, and $a(\hat{X}(t))$, $b(\hat{X}(t))$ are arbitrary functions of $\hat{X}(t)$. The stochastic differential equation can be rewritten as the integral form $\hat{X}(t) = \hat{X}_0 + \int_0^t ds a(\hat{X}(s)) + \int_0^t ds \hat{\xi}(s)b(\hat{X}(s))$, where the last term on the right-hand side (rhs) involves a stochastic integral. In usual stochastic calculus for Gaussian processes, we use one of the following two definitions:

$$\int_0^t ds\hat{\xi}(t) \cdot b(\hat{X}(t)) \equiv \lim_{\Delta t \to +0} \sum_{i=1}^n \Delta t\hat{\xi}(t_i)b(\hat{X}_i), \quad (1)$$

$$\int_0^t ds\hat{\xi}(t) \circ b(\hat{X}(t)) \equiv \lim_{\Delta t \to +0} \sum_{i=1}^n \Delta t\hat{\xi}(t_i) b\left(\frac{\hat{X}_i + \hat{X}_{i+1}}{2}\right), \quad (2)$$

where the symbols \cdot and \circ denote the Itô calculus and the Stratonovich calculus, respectively, and $\Delta t \equiv t/n$, $t_i \equiv i\Delta t$, $\hat{X}_i \equiv \hat{X}(t_i)$. The term $\Delta t \hat{\xi}(t_i)$ is shorthand for $\Delta \hat{W}(t_i) \equiv \hat{W}(t_{i+1}) - \hat{W}(t_i)$, where $\hat{W}(t) \equiv \int_0^t ds \hat{\xi}(s)$ is the Wiener process.

Our strategy to define the new stochastic integral for non-Gaussian processes is the white noise limit of a non-Gaussian colored noise. First, we construct the colored noise by using white noises. Let ϵ be a time constant to characterize the correlation time of the noise, and let $\Delta t \hat{\xi}(t_i)$ be shorthand for $\Delta \hat{L}(t_i) \equiv \hat{L}(t_{i+1}) - \hat{L}(t_i)$, where $\hat{L}(t) \equiv \int_0^t ds \hat{\xi}(s)$ is the Lévy process. We define the colored noise as

$$\Delta t \hat{\xi}_{\epsilon}(t_i) \equiv \frac{1}{l} \sum_{j=0}^{l-1} \Delta t \hat{\xi}(t_{i-j}), \qquad (3)$$

where $l \equiv \epsilon/\Delta t$ is assumed to be an integer. The correlation of the noise satisfies $\langle \hat{\xi}_{\epsilon}(t) \hat{\xi}_{\epsilon}(s) \rangle = 0$ only if $|t - s| \ge \epsilon$. We call this manipulation ϵ smoothing. For example, the white Poisson noise $\hat{\xi}(t) = \sum_i \delta(t - \hat{t}_i)$, where each Poisson flight happens at \hat{t}_i , is used to construct the colored noise as shown in Fig. 1.

Introducing a new symbol *, we propose the following stochastic integral for non-Gaussian processes as a limit of the colored noise:

$$\int_0^t ds \hat{\xi}(t) * f(\hat{X}(t)) \equiv \lim_{\epsilon \to +0} \lim_{\Delta t \to +0} \sum_{i=1}^n \Delta t \hat{\xi}_\epsilon(t_i) f(\hat{X}(t_i)), \quad (4)$$

where f(x) is an arbitrary function. We refer to this integral as the * integral or the * calculus. Correspondingly, we interpret the stochastic differential equation with the * integral as

$$\frac{d\hat{X}(t)}{dt} = a(\hat{X}(t)) + b(\hat{X}(t)) * \xi(t).$$
(5)

The two limits in Eq. (4) are not commutable. In the Itô integral, the limits are taken simultaneously $\Delta t = \epsilon \rightarrow +0$. On the contrary, the limit of $\Delta t \rightarrow +0$ is taken before the limit of $\epsilon \rightarrow +0$ in our formulation. We note that our integral is equivalent to the Stratonovich integral for Gaussian processes [29].

Next, let us discuss the transformation formula from the * integral to the Itô integral. By using Hänggi's functional formula [30,31], we obtain (see the Supplemental Material for a derivation [32])

$$d\hat{L}(t) * f(\hat{X}(t)) = \sum_{n=0}^{\infty} \frac{d\hat{L}^{n+1}(t)}{(n+1)} \cdot \left(\left\{ b(x) \frac{\partial}{\partial x} \right\}^n f(x) \Big|_{x = \hat{X}(t)} \right),$$
(6)

where $b(\hat{X}(t))$ describes the same function in Eq. (5) and $f(\hat{X}(t))$ is an arbitrary function of $\hat{X}(t)$. For Gaussian processes, Eq. (6) reduces to the transformation formula from the Stratonovich integral to the Itô integral because $d\hat{L}^n = 0$ holds for $n \ge 3$. Although other types of ϵ smoothing can be used to construct the colored noise, Eq. (6) does not depend on the way of the ϵ smoothing [33]. We note that Eq. (6) can be regarded as a straightforward generalization of

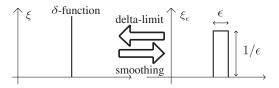


FIG. 1. A schematic of the ϵ smoothing.

the result in Refs. [34,35] in which Eq. (5) has been transformed into the Itô type.

As a simple example, we apply the * calculus to the Black-Scholes equation driven by a Poisson noise [36]

$$\frac{d\hat{X}}{dt} = (-1 + \hat{\xi})\hat{X},\tag{7}$$

where $\hat{\xi} = \hat{\eta} - \lambda I$ with a Poisson noise $\hat{\eta}$ characterized by its intensity I and transition rate λ . The Poisson noise is a typical non-Gaussian noise. In fact, any noise can be decomposed into the combination of Gaussian and Poisson noises [37]. If we define $\hat{\xi}\hat{X}$ on the rhs of Eq. (7) based on the * integral as $\hat{\xi} * \hat{X}$, then the solution of Eq. (7) equals the following quantity: $\hat{Y} = \exp[-t + t]$ $\int_0^t ds \hat{\xi}(s)$, which is the formal solution of the Black-Scholes equation with the ordinary differential calculus. In contrast, if we adopt the Stratonovich integral to define the rhs of Eq. (7), its solution does not equal \hat{Y} . Figure 2 shows the numerical results on $Z \equiv \langle \hat{Y} / \hat{X} \rangle$ for the cases of the * integral and the Stratonovich integral. The ϵ smoothing is performed by the definition of Eq. (3). As I increases, Z becomes different from 1 for the Stratonovich integral due to the non-Gaussian property of the noise. In contrast, the * calculus keeps $Z \approx 1$ independently of the value of *I*. We also note that the result of the Itô calculus is ranged around Z = 5. These results imply that neither Itô nor Stratonovich calculus is obtained as the white noise limit of a colored noise.

Stochastic energetics for non-Gaussian processes.—We now apply the * integral to formulate stochastic energetics for non-Gaussian processes. Let us consider the following underdamped Langevin equations:

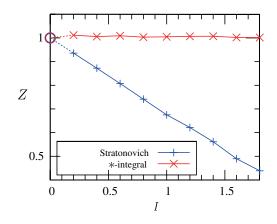


FIG. 2 (color online). Numerical results on the consistency between Eq. (7) and \hat{Y} . We fix the variance of the Poisson noise $\lambda I^2 = 4.0$ and simulate the equation until t = 1.0 with $\epsilon = 0.001$. As *I* increases, the difference between the * integral and the Stratonovich integral becomes significant. In the Gaussian limit of $I \rightarrow 0$, *Z* is expected to equal unity in both calculuses as denoted by an open circle.

$$\frac{d\hat{p}}{dt} = -\frac{\gamma}{m}\hat{p} - \frac{\partial U(\alpha, x)}{\partial x} \bigg|_{x=\hat{x}} + g(\hat{x}, \hat{p}) * \hat{\xi}, \quad \frac{d\hat{x}}{dt} = \frac{\hat{p}}{m}, \quad (8)$$

where $\hat{\xi}$ is a non-Gaussian noise whose mean value is zero, \hat{x} is the position of the particle, \hat{p} is its momentum, and $U(\alpha, x)$ is the potential with an external parameter α , such as the intensity of optical tweezers. If g(x, p) is constant, the noise is called additive; otherwise, it is called multiplicative. It is known that Brownian motion near a wall can be characterized by a multiplicative noise [38]. The detailed balance condition is not assumed in this Letter, and the following results can be applied to athermal systems. We note that the detailed balance condition in athermal systems has been studied in Ref. [39].

Let us first define the thermodynamic quantities for each trajectory. We divide the total energy difference into the following two parts:

$$d\hat{W} = \frac{\partial U}{\partial \alpha} \bigg|_{x=\hat{x}} d\alpha,$$

$$d\hat{Q} = \bigg(-\frac{\gamma \hat{p}^2}{m^2} + \frac{\hat{\xi} * g(\hat{x}, \hat{p})\hat{p}}{m} \bigg) dt,$$
(9)

where \hat{W} is the mechanical work through the parameter α , and \hat{Q} is the energy flow induced by the microscopic degrees of freedom in the environment. The usual heat is included in \hat{Q} . Our formalism has practical utilities for experimental and numerical data analysis of the heat. We refer to \hat{Q} as "heat" for convenience. By using the ordinary chain rule for the * integral, we confirm the first law of thermodynamics

$$d\hat{E} = \frac{\hat{p} * d\hat{p}}{m} + \frac{\partial U}{\partial x} * d\hat{x} + \frac{\partial U}{\partial \alpha} d\alpha = d\hat{Q} + d\hat{W}, \quad (10)$$

where $\hat{E} \equiv \hat{p}^2/2m + U(\alpha, \hat{x})$ is the internal energy of the particle.

We next derive a representation of the average heat flux by using the * calculus. For this purpose, we first write down the Kramers equation for $P(x, p, t) = \langle \hat{P}(x, p, t) \rangle$ with $\hat{P}(x, p, t) = \delta(x - \hat{x}(t))\delta(p - \hat{p}(t))$. The stochastic Liouville equation [40] is given by

$$\frac{\partial}{\partial t}\hat{\mathcal{P}}(x,p,t) + \frac{\partial}{\partial x}\{\dot{x}(t) * \hat{\mathcal{P}}(x,p,t)\} + \frac{\partial}{\partial p}\{\dot{\hat{p}}(t) * \hat{\mathcal{P}}(x,p,t)\} = 0,$$

where the stochastic partial differential equation is regarded as the * calculus. Taking an average of this equation and using the transformation formula Eq. (6), we obtain the generalized Kramers equation

$$\frac{\partial}{\partial t}P = -\frac{\partial}{\partial x} \left(\frac{p}{m}P\right) - \frac{\partial}{\partial p} \left[\left(-\frac{\gamma p}{m} - \frac{\partial U}{\partial x}\right)P + \langle \hat{\xi} * g \, \hat{\mathcal{P}} \rangle \right],\tag{11}$$

where $\langle \hat{\xi} * g \hat{\mathcal{P}} \rangle$ describes the diffusion of the particle. Transforming this diffusion term into the Itô type, we reproduce the ordinary Kramers equation. By introducing

$$J_{x} \equiv \frac{p}{m}P, \qquad J_{p} \equiv \left(-\frac{\gamma p}{m} - \frac{\partial U}{\partial x}\right)P + \langle \hat{\xi} * g \hat{\mathcal{P}} \rangle, \quad (12)$$

we rewrite Eq. (11) as the conservation of the probability $\partial P/\partial t + \partial J_x/\partial x + \partial J_p/\partial p = 0$. Note that the probability fluxes include an infinite number of differentiations if we use the Itô calculus. The probability conservation formula leads to a simple identity of the total derivative for any function $f(x, p, \alpha)$:

$$\left\langle \frac{d}{dt} f(\hat{x}, \hat{p}, \alpha) \right\rangle = \int dx dp \left(\frac{\partial f}{\partial x} J_x + \frac{\partial f}{\partial p} J_p \right) + \dot{\alpha} \left\langle \frac{\partial f}{\partial \alpha} \right\rangle.$$
(13)

Taking $f(x, p, \alpha)$ as $E(x, p, \alpha)$, we derive that the heat satisfies the formula of the average of heat flux

$$\left\langle \frac{d\hat{Q}}{dt} \right\rangle = \int dx dp \left(\frac{\partial E}{\partial x} J_x + \frac{\partial E}{\partial p} J_p \right). \tag{14}$$

We note that we can straightforwardly apply the * calculus to the overdamped Langevin equation.

Heat measurement formula.—In the case of the underdamped Langevin equation driven by an additive non-Gaussian noise, the transformation formula Eq. (6) can be reduced to

$$d\hat{Q} = -\frac{\gamma \hat{p}^2}{m^2} dt + d\hat{L} * \frac{\hat{p}}{m} = -\frac{\gamma \hat{p}^2}{m^2} dt + d\hat{L} \cdot \frac{\hat{p}}{m} + \frac{(d\hat{L})^2}{2}.$$
 (15)

This formula can be applied to the measurements of the heat in experiments because Eq. (6) includes the noise term only up to the second order. The term $(d\hat{L})^2$ is not deterministic but stochastic, contrary to the cases of the Gaussian noise, in which $(d\hat{L})^2$ can be replaced by $\sigma^2 dt$ with the variance σ . We note that the formula for the heat measurement becomes more complicated for multiplicative noises. We also note that the heat measurement formula for the overdamped Langevin equation is not simple even for additive noises, where higher order cumulants appear for the cases of a nonharmonic potential [33].

A model of ATP reception.—To demonstrate how a non-Gaussian feature appears in a stochastic process, let us analyze a Brownian particle in an ATP bath. When the particle receives an ATP, the particle suddenly moves. We assume that the particle obeys the overdamped Langevin equation under a nonharmonic potential $U(x) = (k/2)x^2 + (\epsilon/4)x^4$ with small ϵ . The system is driven by an additive Poisson noise whose transition rate $P(x \rightarrow y)$ is given by $P(x \rightarrow y) = \lambda/2$ (if $x - y = \pm I/\gamma$), 0 (otherwise), where I is the intensity of the Poisson noise and γ is a friction constant. We note that the detailed balance condition is violated in this model. The dimensionless Langevin equation of this system is given by

$$\frac{d\hat{X}}{d\tau} = -\hat{X} - \tilde{\epsilon}\hat{X}^3 + \hat{\xi}, \qquad d\hat{L} = \hat{\xi}d\tau, \qquad (16)$$

$$\langle d\hat{L}^n \rangle = \begin{cases} 0 & (n \text{ odd}) \\ (t_p/t_s)^{n/2-1} d\tau & (n \text{ even}) \end{cases},$$
(17)

where we introduced the characteristic constants and dimensionless parameters as $t_s = \gamma/k$, $t_p = 1/\lambda$, $x_s = (I/\gamma)\sqrt{(t_s/t_p)}$, $\tilde{\epsilon} = x_s^2 \epsilon/k$, $\hat{x} = x_s \hat{X}$, and $t = t_s \tau$. Note that t_s and t_p are the characteristic time scales of the relaxation of the system and the Poisson noise, respectively, and therefore t_p/t_s characterizes non-Gaussian effects. By analyzing this model, we demonstrate that the * integral is consistent with the first law of thermodynamics and that the non-Gaussian effects are relevant for $t_p \sim t_s$.

We first demonstrate that the first law of thermodynamics is consistent with the * calculus in this system. Let us define the three types of dimensionless energies $\tilde{U} \equiv \frac{\hat{X}^2}{2} + \frac{\epsilon \hat{X}^4}{4}$, $\tilde{U}^* \equiv \int_0^{\tau} d\hat{X}(s) * \frac{\partial \tilde{U}}{\partial x}$, $\tilde{U}^S \equiv \int_0^{\tau} d\hat{X}(s) \circ \frac{\partial \tilde{U}}{\partial x}$, where \tilde{U} is the total potential energy, \tilde{U}^* is the heat with the * calculus, and \tilde{U}^S is that with the Stratonovich calculus. We note that the work is zero in this case. Figure 3 shows the time evolution of the three quantities without taking the ensemble average, where \tilde{U}^* is consistent with the first law of thermodynamics, while \tilde{U}^S is not.

We next derive the condition where non-Gaussian effects are relevant. The average of the energy in the steady state can be obtained for small ϵ as $\lim_{\tau \to \infty} \langle \tilde{U} \rangle = 1/4 - 3\tilde{\epsilon}/16 - (\tilde{\epsilon}/16)(t_p/t_s)$. This implies that we cannot ignore the non-Gaussian effect for $t_p \approx t_s$, while the non-Gaussian effect vanishes for $t_s \gg t_p$. In fact, t_p is the relaxation time in which the Poisson noise converges to a Gaussian noise according to the central limit theorem. For $t_p \approx t_s$, the system evolves before the relaxation, and therefore we cannot replace the Poisson noise by a Gaussian noise. In contrast, we can adiabatically eliminate the non-Gaussian effect in the Poisson process for $t_s \gg t_p$.

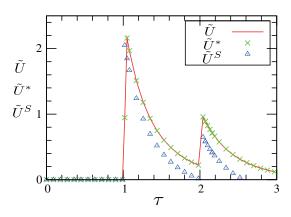


FIG. 3 (color online). The check of the first law of thermodynamics through the numerical solution of Eq. (16) with the intensity $I = \pm 2.0$ where the Poisson noises are added at $\tau =$ 1.0 and $\tau = 2.0$. The result of \tilde{U}^* based on the * calculus agrees with the total energy \tilde{U} , while \tilde{U}^S based on the Stratonovich calculus is different from \tilde{U} .

Conclusion.—In this Letter, we have developed the stochastic energetics of small thermodynamic systems driven by a non-Gaussian noise by introducing the new stochastic integral Eq. (4), which we refer to as the * integral. The investigation of the second law of thermodynamics and fluctuation theorem for non-Gaussian processes is a future issue, in which the * calculus would play an important role.

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