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Abstract
We demonstrate that a Langevin equation that describes the motion of a
Brownian particle under non-equilibrium conditions can be exactly transformed
to a special equation that explicitly exhibits the response of the velocity to a
time-dependent perturbation. This transformation is constructed on the basis
of an operator formulation originally used in nonlinear perturbation theory for
differential equations by extending it to stochastic analysis. We find that the
expression obtained is useful for the calculation of fundamental quantities of
the system, and that it provides a physical basis for the decomposition of the
forces in the Langevin description into effective driving, dissipative and random
forces in a large-scale description.

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1. Introduction

Owing to technological advances in the methods of manipulating systems on sub-micrometre
length scales in aqueous solution, there is increased interest in studying the non-equilibrium
nature of such small systems. Recent studies have yielded several universal relations, including
the fluctuation theorem [1], the Jarzynski equality [2] and the Hatano–Sasa non-equilibrium
steady state equality [3], and the validity of these relations has been verified experimentally
in small systems consisting of beads and bead-RNA complexes [4–6]. In addition to the
verification of these equalities, there is an interesting experimental study providing new
information concerning the nature of non-equilibrium systems, in which the velocity response
to an external perturbation and the correlation of the corresponding fluctuations were measured
in a bead system [7]. We should also mention that there has been a substantial progress in
understanding stochastic resonance [8, 9].

Although great progress has been made in the experimental investigation of such small systems, direct measurements have been possible only for kinematic quantities, such as the position of a bead. Given this situation, in order to elucidate the mechanics of small systems, it is necessary to extract information regarding mechanical quantities, such as 'force' and 'energy', from kinematic quantities. However, this task is not easily accomplished in general. For instance, consider the problem of guessing the equation of motion of a motor protein on the basis of experimental results. It can then be understood why it is difficult to determine an effective potential for the centre of mass and to evaluate the size of dissipation effects, because neither a canonical distribution nor a fluctuation–response relation exists for non-equilibrium systems. (By contrast, these can be utilized to determine an effective potential and a dissipation strength near equilibrium states.)

In this paper, we study a non-equilibrium Langevin system for the purpose of developing a new theoretical method to extract information regarding mechanical quantities in small systems. Specifically, we attempt to re-express a Langevin equation in terms of directly measurable quantities. Here, let us recall that, for differential equations, there exists a theoretical method by which, for example, a Rayleigh equation that describes nonlinear oscillations can be transformed perturbatively into a simple equation displaying the observed frequency [10]. Following this idea, it might be useful if we could transform a Langevin equation into a special form that makes mechanical properties manifest. Specifically, motivated by a recent phenomenological study of energy efficiency [11], we regard the response to a time-dependent perturbative force as a key property that connects kinematic and mechanical quantities.

Here, we point out that a Langevin equation is equivalent to the corresponding Fokker–Planck equation as long as we consider statistical properties. However, when we study problems related to force and energy, analysis of a Langevin equation is more appropriate, because it can be regarded as an equation of force balance. Furthermore, physical quantities for a single trajectory, which are often observed in bio-mechanical systems [12], can be described only by a Langevin equation. For these reasons, we seek a useful representation of a Langevin equation rather than a Fokker–Planck equation.

Explicitly, we study the simple one-dimensional Langevin equation

$$\gamma \dot{x}(t) = f - U'(x(t)) + \xi(t) + \varepsilon f_{\mathrm{p}}(t). \tag{1}$$

Here, γ is a friction constant, f is a constant driving force, $U(x)$ is a periodic potential of period ℓ and the prime denotes differentiation. Also, $\xi(t)$ is Gaussian white noise satisfying

$$\langle \xi(t)\xi(s) \rangle = 2\gamma T \delta(t - s), \tag{2}$$

where $\langle \cdots \rangle$ denotes the average over all noise histories. (See [13, 14] for discussion of the physical basis of this equation in the case $\varepsilon = 0$.) The term $\varepsilon f_{\mathrm{p}}(t)$ with sufficiently small ε represents a perturbation force we use to investigate the response of the system. An initial condition $x(t_0) = x_0$ is given at $t = t_0$, and we often take the limit $t_0 \to -\infty$. In the argument below, we denote the average over all noise histories in the limit $t_0 \to -\infty$ as $\langle \cdots \rangle_\varepsilon$. Under these conditions, there exists the time-dependent distribution function $p_\infty(\theta, t)$, such that the relation

$$\langle A(x(t)) \rangle_\varepsilon = \int_0^\ell \mathrm{d}\theta \, A(\theta) p_\infty(\theta, t) \tag{3}$$

is satisfied for any ℓ-periodic function $A(\theta)$. Note that $p_\infty(\theta, t)$ can be expanded in the form

$$p_\infty(\theta, t) = p_{\mathrm{st}}(\theta) + \varepsilon p^{(1)}(\theta, t) + O(\varepsilon^2). \tag{4}$$

With the above preparation, in section 2, we prove the following theorem.

Theorem. *Under the condition* $t_0 \to -\infty$, *equation (1) can be transformed into the form*

$$\int_0^\infty \mathrm{d}s\, L(s)(\dot{x}(t-s) - v_\mathrm{s}) = \int_0^\infty \mathrm{d}s\, L(s)\zeta(t-s) + \xi(t) + \varepsilon f_\mathrm{p}(t), \tag{5}$$

where $v_\mathrm{s} \equiv \langle \dot{x}(t) \rangle_0$ *is the steady-state velocity. The function* $L(s)$ *here is determined by the system parameters* γ, f, $U(x)$ *and* T, *and is independent of* ε. $L(s)$ *is determined so that it satisfies the causality property, i.e.,* $L(t) = 0$ *for* $t < 0$. *The function* $\zeta(t)$ *depends on* $\{x(s)\}_{t_0 \leqslant s \leqslant t}$, $\{\xi(s)\}_{t_0 \leqslant s \leqslant t}$ *and* $\{f_\mathrm{p}(s)\}_{t_0 \leqslant s \leqslant t}$, *and most importantly it satisfies the relation*

$$\langle \zeta(t) \rangle_\varepsilon = O(\varepsilon^2). \tag{6}$$

These functions, $L(s)$ *and* $\zeta(s)$, *are determined from the set of eigenfunctions of the Fokker–Planck operator corresponding to the Langevin equation (1), as explained in section 2.3.*

We now explain the physical significance of this theorem. First, note that (5) is equivalent to the form

$$\dot{x}(t) - v_\mathrm{s} = \zeta(t) + \int_0^\infty \mathrm{d}s\, R(s)(\xi(t-s) + \varepsilon f_\mathrm{p}(t-s)). \tag{7}$$

Here, the quantity $R(t)$ is determined from $L(t)$ through the relation

$$\tilde{R}(\omega) = \tilde{L}(\omega)^{-1}, \tag{8}$$

where $\tilde{R}(\omega)$ and $\tilde{L}(\omega)$ are the Fourier transforms of $R(t)$ and $L(t)$. $R(t)$ for $t > 0$ is obtained by the inverse Fourier transform and we also require the causality as $R(t) = 0$ for $t < 0$. Throughout this paper, we use similar notation, with the Fourier transform of an arbitrary function $A(t)$ given by

$$\tilde{A}(\omega) = \int_{-\infty}^\infty \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} A(t). \tag{9}$$

Then, the average of (7) becomes

$$\langle \dot{x}(t) \rangle_\varepsilon - v_\mathrm{s} = \varepsilon \int_0^\infty \mathrm{d}s\, R(s) f_\mathrm{p}(t-s) + O(\varepsilon^2). \tag{10}$$

This equation characterizes the linear response of the velocity to the perturbation. We therefore call $R(s)$ a 'response function'. Its Fourier transform, $\tilde{R}(\omega)$, is called the 'dynamic susceptibility'. Expression (7), which is equivalent to the original equation of motion (1), explicitly represents the response to a perturbation.

Next, we show how expression (5) is related to the problem of force decomposition in a large-scale description. Let us express the force acting on the particle at time t as

$$\phi(t) \equiv f - U'(x(t)) \tag{11}$$

and consider a finite time average of $\phi(t)$. For convenience, we express the finite time average of a quantity $A(t)$ as

$$\bar{A}_\tau(t) = \frac{1}{\tau} \int_t^{t+\tau} \mathrm{d}s\, A(s). \tag{12}$$

From (1), (5), (11) and (12), we find

$$\bar{\phi}_\tau(t) = \gamma \frac{x(t+\tau) - x(t)}{\tau} + \int_0^\infty \mathrm{d}s\, L(s)\bar{\zeta}_\tau(t-s)$$
$$- \int_0^\infty \mathrm{d}s\, L(s)\left(\frac{x(t-s+\tau) - x(t-s)}{\tau} - v_\mathrm{s} \right). \tag{13}$$

We now assume that τ is sufficiently larger than the inverse of the smallest decay rate of $L(s)$. Then, because $\bar{A}_\tau(t)$ varies slowly with respect to t, (13) becomes

$$\bar{\phi}_\tau(t) \simeq \tilde{L}(0)v_s - (\tilde{L}(0) - \gamma)\frac{x(t+\tau) - x(t)}{\tau} + \tilde{L}(0)\bar{\xi}_\tau(t). \tag{14}$$

This expression implies that a time-averaged force $\bar{\phi}_\tau(t)$ can be decomposed into a driving force (the first term), a dissipative force (the second term) and a random force (the third term). In [15], the force decomposition for a large-scale description with (1) is investigated, and it is shown that the condition

$$\lim_{\tau \to \infty} \tau \langle \bar{\zeta}_\tau \bar{\xi}_\tau \rangle_0 = 0 \tag{15}$$

uniquely determines the force decomposition of the type given in (14). In other words, only the component orthogonal to $\bar{\xi}_\tau$ is regarded as a random component of $\bar{\phi}_\tau$ in such a description. In section 2.4, we confirm that this orthogonality condition is satisfied. Actually, we have arrived at expression (5) by seeking a definition of $\zeta(t)$ for which (15) holds. In this sense, (15) was the guiding principle used in obtaining the transformation yielding (5) from (1).

In section 3, we demonstrate that expression (7) is useful for calculating fundamental statistical quantities. As already stated, the susceptibility $\tilde{R}(\omega)$ is obtained as the Fourier transform of $R(t)$. In appendix A, we provide a consistency check of our theory by comparing this quantity $\tilde{R}(\omega)$ with an expression that is obtained directly from the definition of the dynamic susceptibility. Furthermore, the Fourier transform $\tilde{C}(\omega)$ of the time correlation of velocity fluctuations,

$$C(t) \equiv \langle (\dot{x}(t) - v_s)(\dot{x}(0) - v_s) \rangle_0, \tag{16}$$

can also be calculated directly from (7). In particular, for the case $\omega = 0$, we can derive the following formulae:

$$\tilde{R}(0) = \frac{\ell}{\gamma}\frac{\int_0^\ell d\theta\, I_-(\theta)I_+(\theta)}{\left(\int_0^\ell dx\, I_-(\theta)\right)^2}, \tag{17}$$

$$\frac{\tilde{C}(0)}{2} = \frac{T}{\gamma}\ell^2\frac{\int_0^\ell d\theta\, I_-(\theta)I_+(\theta)^2}{\left(\int_0^\ell d\theta\, I_-(\theta)\right)^3}, \tag{18}$$

where

$$I_\pm(\theta) = \int_0^\ell d\theta'\, e^{\pm\beta U(\theta) \mp \beta U(\theta \mp \theta') - \beta f\theta'}, \tag{19}$$

with $\beta \equiv 1/T$. The key technical lemma used in the derivations of the above relations is proved in appendix B.

We note that $\tilde{R}(0)$ is equal to the differential mobility, dv_s/df, and that expression (17) was calculated from the functional form of $v_s(f)$ given in [16]. Also, $\tilde{C}(0)/2$ is equal to the diffusion constant D defined by

$$D \equiv \lim_{t \to \infty} \frac{1}{2t}\langle (x(t) - x(0) - v_s t)^2 \rangle_0. \tag{20}$$

Expression (18) was first derived in [14] employing a recursion formula that is established in the theory of stochastic processes. Subsequently, the same expression was obtained in a perturbation theory treatment applied to the Fokker–Planck equation corresponding to (1) [16]. The method of derivation used in the present work is different from those used in the previous studies.

Furthermore, from the correspondence of $\tilde{R}(0)$ with $\mathrm{d}v_\mathrm{s}/\mathrm{d}f$ and from the definition of D in (20), the nature of each term in the force decomposition (14) is clearly understood. By substituting (14) into the τ-averaged form of (1), we obtain a large-scale description of the Langevin equation:

$$\tilde{L}(0)\frac{x(t+\tau)-x(t)}{\tau} = \tilde{L}(0)v_\mathrm{s} + \bar{\xi}_\tau(t) + \tilde{L}(0)\bar{\zeta}_\tau(t). \tag{21}$$

The effective dissipation coefficient, $\tilde{L}(0)$, is the inverse of the differential mobility $\tilde{R}(0)$ as explained in (8). The magnitude of the fluctuating forces, $\langle(\bar{\xi}_\tau(t)+\tilde{L}(0)\bar{\zeta}_\tau(t))^2\rangle_0$, is expressed in terms of the diffusion constant as $2D/\tilde{R}(0)^2$, which provides the renormalization of the bare noise intensity $2\gamma T$. These quantities are obtained by use of the explicit expressions given in (17) and (18).

2. Proof of theorem

2.1. Operator formulation

In order to make the argument mathematically clearer, we express the Langevin equation (1) as

$$\gamma\,\mathrm{d}x(t) = \{f - U'(x(t))\}\,\mathrm{d}t + \sqrt{2\gamma T}\,\mathrm{d}w(t) + \varepsilon f_\mathrm{p}(t)\,\mathrm{d}t, \tag{22}$$

where $w(t)$ represents a Wiener process [17]. Let $A(x)$ be an arbitrary function of x. Then, Itô's formula gives

$$\mathrm{d}A(x(t)) = \frac{F(x(t))}{\gamma}A'(x(t))\,\mathrm{d}t + \frac{T}{\gamma}A''(x(t))\,\mathrm{d}t + \sqrt{\frac{2T}{\gamma}}A'(x(t))\cdot\mathrm{d}w + \frac{1}{\gamma}\varepsilon f_\mathrm{p}(t)A'(x(t))\,\mathrm{d}t, \tag{23}$$

where

$$F(x) \equiv f - U'(x). \tag{24}$$

Here, $\cdot$ represents the product in the Itô interpretation. In conventional notation, this is written as

$$\frac{\mathrm{d}A(x(t))}{\mathrm{d}t} = \Lambda A(x)|_{x=x(t)} + A'(x(t))\cdot\frac{1}{\gamma}(\xi(t) + \varepsilon f_\mathrm{p}(t)), \tag{25}$$

where

$$\Lambda \equiv \frac{F(x)}{\gamma}\frac{\partial}{\partial x} + \frac{T}{\gamma}\frac{\partial^2}{\partial x^2}. \tag{26}$$

We can express the solution of (25) in the form

$$A(x(t)) = \mathcal{G}(t)A(x)|_{x=x_0} \tag{27}$$

by introducing a time-dependent operator, $\mathcal{G}(t)$, that does not depend on $A(x)$. Substituting (27) into (25), we obtain an equation for $\mathcal{G}(t)$ as

$$\frac{\mathrm{d}\mathcal{G}(t)}{\mathrm{d}t} = \mathcal{G}(t)\Lambda + \mathcal{G}(t)\frac{\partial}{\partial x}\cdot\frac{1}{\gamma}(\xi(t) + \varepsilon f_\mathrm{p}(t)). \tag{28}$$

With the initial condition $\mathcal{G}(t_0) = 1$, the formal solution of this equation is derived as

$$\mathcal{G}(t) = \mathrm{e}^{(t-t_0)\Lambda} + \int_0^{t-t_0}\mathrm{d}s\,\mathcal{G}(t-s)\frac{\partial}{\partial x}\,\mathrm{e}^{s\Lambda}\cdot\frac{1}{\gamma}(\xi(t-s) + \varepsilon f_\mathrm{p}(t-s)). \tag{29}$$

Thus, because the force acting on the particle at time t is given by

$$
\begin{aligned}
\phi(t) &= F(x(t)) \\
&= \mathcal{G}(t)F(x)|_{x=x_0},
\end{aligned}
\tag{30}
$$

we obtain

$$
\phi(t) = \mathrm{e}^{(t-t_0)\Lambda}F(x)|_{x=x_0} + \int_0^{t-t_0} \mathrm{d}s\, \frac{\xi(t-s) + \varepsilon f_{\mathrm{p}}(t-s)}{\gamma} \cdot \frac{\partial}{\partial x}\, \mathrm{e}^{s\Lambda} F(x)|_{x=x(t-s)},
\tag{31}
$$

where we have used (27) in the derivation of the second term on the right-hand side.

In this way, we have reformulated the original nonlinear stochastic differential equation in terms of the operator Λ. We note that a theoretical framework for carrying out such a reformulation in the case of differential equations was developed through application of nonlinear perturbation theory [18]. Also, analysis based on the 'microscopic distribution function' [19] is essentially the same as the present formulation.

2.2. Preparation of functional space

In order to make our investigation of (31) concrete, we introduce a functional space, $\mathcal{H}$, consisting of all complex-valued, square integrable, periodic functions of θ on the interval $0 \leqslant \theta \leqslant \ell$. We endow this space with the inner product

$$
(h_1, h_2) = \int_0^\ell \mathrm{d}\theta\, h_1^*(\theta) h_2(\theta),
\tag{32}
$$

for $h_1, h_2 \in \mathcal{H}$, where $*$ denotes complex conjugation. All the eigenvalues, $-\lambda_j$, and the corresponding eigenfunctions, $\Phi_j(\theta)$, of the operator Λ in $\mathcal{H}$ are determined by the equation

$$
\Lambda \Phi_j(\theta) = -\lambda_j \Phi_j(\theta),
\tag{33}
$$

where the index $j = 0, \pm1, \pm2, \ldots$ is determined by the relations $\lambda_j = \lambda_{-j}^*$ and $\lambda_0 = 0 < \mathrm{Re}(\lambda_{\pm1}) < \mathrm{Re}(\lambda_{\pm2}) < \cdots$ holding among their eigenvalues. When a complex eigenvalue happens to be degenerate, the corresponding labelling is modified appropriately.

Because Λ given in (26) is not a Hermitian operator on $\mathcal{H}$, it is convenient to introduce the adjoint operator of Λ through the relation

$$
(\mathcal{L}_{\mathrm{FP}}h_1, h_2) \equiv (h_1, \Lambda h_2),
\tag{34}
$$

where $\mathcal{L}_{\mathrm{FP}}$ is the Fokker–Planck operator:

$$
\mathcal{L}_{\mathrm{FP}} = -\frac{1}{\gamma}\frac{\partial}{\partial\theta}F(\theta) + \frac{T}{\gamma}\frac{\partial^2}{\partial\theta^2}.
\tag{35}
$$

Note that the set of eigenvalues of $\mathcal{L}_{\mathrm{FP}}$ is identical to that of Λ. Then, we denote the eigenfunctions of $\mathcal{L}_{\mathrm{FP}}$ by $\Psi_j(\theta)$ and choose their labelling so that we have

$$
\mathcal{L}_{\mathrm{FP}}\Psi_j(\theta) = -\lambda_j^* \Psi_j(\theta).
\tag{36}
$$

We can choose these eigenfunctions such that the following hold:

$$
\int_0^\ell \mathrm{d}\theta\, \Psi_i^*(\theta)\Phi_j(\theta) = \delta_{ij},
\tag{37}
$$

$$
\sum_{j=-\infty}^\infty \Psi_j^*(\theta)\Phi_j(\theta') = \delta(\theta - \theta').
\tag{38}
$$

In particular, we determine the normalization factor for the zero eigenfunctions

$$\Psi_0(\theta) = p_{st}(\theta), \tag{39}$$

$$\Phi_0(\theta) = 1. \tag{40}$$

Because $F(\theta) \in \mathcal{H}$, we can expand $F(\theta)$ in the form

$$F(\theta) = \sum_{j=-\infty}^{\infty} (\Psi_j, F)\Phi_j(\theta). \tag{41}$$

Here, the following relation is easily confirmed:

$$(\Psi_0, F) = \gamma v_s. \tag{42}$$

Then, from (31) and (41), we obtain

$$\phi(t) = \gamma v_s + b(t) + \int_0^{t-t_0} ds \, (\xi(t-s) + \varepsilon f_p(t-s)) \cdot K(s, x(t-s)), \tag{43}$$

with

$$b(t) \equiv \sum_{j=-\infty, j \neq 0}^{\infty} (\Psi_j, F) \, e^{-\lambda_j (t-t_0)} \Phi_j(x_0) \tag{44}$$

and

$$K(s, \theta) \equiv \frac{1}{\gamma} \sum_{j=-\infty}^{\infty} e^{-s\lambda_j} (\Psi_j, F)\Phi'_j(\theta) \tag{45}$$

for $s > 0$ and $K(s, \theta) \equiv 0$ for $s < 0$. Note that $b(t)$ satisfies the relation

$$\lim_{t_0 \to -\infty} b(t) = 0. \tag{46}$$

2.3. Key step

We decompose $K(s, \theta)$ into two parts as

$$K(s, \theta) = K_0(s) + K_\perp(s, \theta), \tag{47}$$

where we have

$$K_0(s) \equiv (\Psi_0, K(s, \cdot)) \tag{48}$$

for $s > 0$ and $K_0(s) \equiv 0$ for $s < 0$. We choose this decomposition in order to satisfy the relation

$$\langle K_\perp(s, x(t)) \rangle_0 = \int_0^{\ell} d\theta \, p_{st}(\theta) K_\perp(s, \theta)$$

$$= 0. \tag{49}$$

Indeed, this equality can be derived from (37) and (39). Now, defining the quantity

$$\zeta(t) \equiv \frac{1}{\gamma} \int_0^{t-t_0} ds \, (\xi(t-s) + \varepsilon f_p(t-s)) \cdot K_\perp(s, x(t-s)), \tag{50}$$

we rewrite $\phi(t)$ as

$$\phi(t) = \gamma v_s + b(t) + \int_0^{t-t_0} ds \, K_0(s)(\gamma \dot{x}(t-s) - \phi(t-s)) + \gamma \zeta(t). \tag{51}$$

Here, we introduce

$$\varphi(t) \equiv \phi(t) - \gamma v_\mathrm{s}, \tag{52}$$

$$\Delta(t) \equiv \dot{x}(t) - v_\mathrm{s} \tag{53}$$

and take the limit $t_0 \to -\infty$. The Fourier transform of (51) then yields

$$\tilde{\varphi}(\omega) = \tilde{K}_0(\omega)(\gamma \tilde{\Delta}(\omega) - \tilde{\varphi}(\omega)) + \gamma \tilde{\zeta}(\omega). \tag{54}$$

From this, we derive

$$\tilde{\varphi}(\omega) = \frac{1}{1 + \tilde{K}_0(\omega)}[\tilde{K}_0(\omega)\gamma \tilde{\Delta}(\omega) + \gamma \tilde{\zeta}(\omega)]. \tag{55}$$

The inverse Fourier transform of this expression yields

$$\phi(t) = \gamma \dot{x}(t) - \int_0^\infty \mathrm{d}s\, L(s)(\dot{x}(t - s) - v_\mathrm{s}) + \int_0^\infty \mathrm{d}s\, L(s)\zeta(t - s), \tag{56}$$

with

$$L(t) = \int_{-\infty}^\infty \frac{\mathrm{d}\omega}{2\pi}\, \mathrm{e}^{-\mathrm{i}\omega t}\, \frac{\gamma}{1 + \tilde{K}_0(\omega)} \tag{57}$$

for $t > 0$ and $L(t) = 0$ for $t < 0$. Then, recalling (11), we find that (56) leads to expression (5).

Next, using (3) and (4), we find that $\zeta(t)$ defined by (50) satisfies

$$\langle \zeta(t) \rangle_\varepsilon = \frac{\varepsilon}{\gamma} \int_0^\infty \mathrm{d}s\, f_\mathrm{p}(t - s)\langle K_\perp(s, x(t - s)) \rangle_0 + O(\varepsilon^2), \tag{58}$$

where we have used the Itô interpretation. Finally, from (49), we derive (6).

2.4. Remark

As seen in the above discussion, the proper definition of ζ is essential to obtain (6). We arrived at definition (50) in the following way. Intuitively, ζ corresponds to what is in some sense the 'random' part of the force $\phi(t)$ for the case $\varepsilon = 0$. With this in mind, we assume the following conditions:

$$\langle \zeta(t) \rangle_0 = 0, \tag{59}$$

$$\langle \zeta(t)\xi(t') \rangle_0 = 0. \tag{60}$$

Condition (59) is obviously necessary, and condition (60) is inspired by the orthogonality condition (15) reported in [15]. From definition (50), it is readily confirmed

$$\langle \zeta(t)\xi(t') \rangle_0 = \frac{1}{\gamma} \int_0^\infty \mathrm{d}s\, \langle K_\perp(s, x(t - s)) \rangle_0 \langle \xi(t - s)\xi(t') \rangle$$

$$= 0, \tag{61}$$

where (49) has been used in the last line. It should be noted that condition (60) is satisfied regardless of the interpretation of the multiplication between $\zeta(t)$ and $\xi(t)$. Then, guided by condition (60), we find definition (50), and this leads to the proof of (6).

3. Application

First, we consider the response function $R(t)$. From (45), (48) and (57), we obtain the following expression of the dynamic susceptibility:

$$\tilde{R}(\omega) = \frac{1}{\gamma} \left[1 + \frac{1}{\gamma} \sum_{j=-\infty}^{\infty} \frac{(\Psi_j, F)}{\lambda_j - i\omega} (\Psi_0, \Phi'_j) \right]. \tag{62}$$

Replacement of the infinite sum on the right-hand side of (62) with a finite sum enables us to calculate $\tilde{R}(\omega)$ within a required precision because the contribution of the term with large $|j|$ to the right-hand side in (62) becomes of the order of $|j|^{-2}$ for sufficiently large $|j|$. The response function $R(t)$ is obtained from the inverse Fourier transform.

Next, note that the most important quantity characterizing the statistical properties of fluctuations described by (1) might be the velocity correlation function (16). For the equilibrium case, $f = 0$, as a result of the detailed balance condition, $C(t)$ is determined by $R(t)$ through the fluctuation–response relation. However, for non-equilibrium cases, there is no such relation. Thus, we need to derive an expression of $C(t)$ independently of $R(t)$.

Substituting (50) into (7), we find that it is convenient to define

$$M(s, \theta) \equiv \frac{1}{\gamma} K_\perp(s, \theta) + R(s). \tag{63}$$

We then obtain

$$C(t) = 2\gamma T \int_0^\infty ds \langle M(s, \theta) M(s - t, \theta) \rangle_0, \tag{64}$$

by use of (2). Noting that $C(t) = C(-t)$ and that $M(t, \theta) = 0$ for $t < 0$, we calculate

$$\tilde{C}(\omega) = 2\gamma T \langle |\tilde{M}(\omega, \theta)|^2 \rangle_0$$

$$= \frac{2T}{\gamma} \left(\Psi_0, \left| 1 + \frac{1}{\gamma} \sum_{j=-\infty}^{\infty} \frac{(\Psi_j, F)}{\lambda_j - i\omega} \Phi'_j \right|^2 \right). \tag{65}$$

With this expression, $\tilde{C}(\omega)$ can be calculated with a required precision for the same reason as in the case of $\tilde{R}(\omega)$. The correlation function $C(t)$ is obtained from the inverse Fourier transform. We remark that the result (65) does not depend on the manner in which we interpret the multiplication between $\dot{x}(t)$ and $\dot{x}(0)$ in (16).

Here, we derive more compact expressions for $\tilde{R}(0)$ and $\tilde{C}(0)$. First, for later convenience, we define

$$V(\theta) \equiv U(\theta) - f\theta. \tag{66}$$

Obviously, $F = -V'$. Then, it is easy to confirm the equality

$$e^{\beta f\theta} \int_0^\ell d\theta' \, e^{-\beta U(\theta - \theta') - \beta f\theta'} = \int_0^\ell d\theta' \, e^{-\beta V(\theta')} - (1 - e^{\beta f\ell}) \int_0^\theta d\theta' \, e^{-\beta V(\theta')}. \tag{67}$$

Using this, the expression of $p_{st}(\theta)$ obtained by solving the equation $\mathcal{L}_{FP} p_{st}(\theta) = 0$ with standard techniques (see, e.g., [13]) can be transformed into the form

$$p_{st}(\theta) = \frac{I_-(\theta)}{\int_0^\ell d\theta' I_-(\theta')}. \tag{68}$$

Equality (67) also allows us to prove the relation

$$1 - \frac{1}{\gamma} \sum_{j=-\infty}^{\infty} \frac{(\Psi_j, V')}{\lambda_j} \Phi'_j(\theta) = \ell \frac{I_+(\theta)}{\int_0^\ell d\theta I_-(\theta)}. \tag{69}$$

(The proof of (69) is given in appendix B.) Then, substituting (68) and (69) into both (62) and (65) with $\omega = 0$, we obtain (17) and (18).

Before ending this section, we discuss the similarities and the differences between our formulation and the standard analysis on the basis of the Fokker–Planck equation. We first emphasize that calculation of statistical quantities by use of (7) is in principle equivalent to that using the Fokker–Planck equation that corresponds to the Langevin equation (1). In practice, we should use either formulation depending on the character of the concerned quantity. For example, statistics of an arbitrary function of $x(t)$ can be more easily calculated in the Fokker–Planck formulation. A class of quantities such as the multiple-time correlation functions of $x(t) - x(0)$, which is calculated in the Fokker–Planck formulation, can also be easily calculated from (7) by considering products of the x variables and subsequently averaging over statistical realizations.

On the other hand, as an advantage of our formulation, the calculation of statistical quantities involving $\dot{x}(t)$ is facilitated by use of our formulation. For example, as seen in the above argument, the time correlation function of the velocity fluctuations, $C(t)$, can be easily calculated in our formulation, while such a calculation seems rather difficult, but not impossible, in the Fokker–Planck formulation. Also, owing to the form of (7), it provides a powerful tool to find a statistical quantity connected to the response function. Recently, an illuminating example using this advantage has been demonstrated in [20], in which the steady heat flux has been expressed in terms of the violation of fluctuation–dissipation relation.

4. Concluding remarks

In this paper, we presented the exact transformation of the Langevin equation (1) to (5) as an example. Our theory may provide a novel way of understanding the 'force' in a Langevin system as well as a new method to calculate $\tilde{R}(\omega)$ and $\tilde{C}(\omega)$ simultaneously. Due to the general nature of the argument used in its derivation, our theory can be applied to various stochastic systems. For example, it is straightforward to study a Büttiker model [21] using our theory. For other models, with time-dependent potentials [22–25], some additional techniques must be designed in order to construct a special expression that explicitly exhibits a response function. We will report such studies in a separate paper.

The connection of the theory presented here to experimental studies is most important. As an example, suppose that we have an experimental system consisting of a small particle exhibiting a fluctuating movement on a one-dimensional track and that the mechanics of the system is under investigation. Then, the function $L(s)$ can be determined from the response to a time-dependent perturbation by using (8) and (10), and the statistical properties of $\zeta(t)$ can be determined from the time correlation of $\dot{x}(t)$ by using (50), (63) and (65). Given this $L(t)$ and the statistics of $\zeta(t)$, we can write an equation of the form (5) where $\zeta(t)$ is replaced with artificial random noise satisfying the observed statistics. Such an equation can be considered as the equation of motion for this system provided that the history dependence of $\zeta(t)$ is negligible. Although, strictly speaking, ζ depends on the history of x, this description may provide a good starting point for the construction of a phenomenological theory [11].

The idea of re-expressing differential equations reminds us of the normal form theory, whose goal is to transform the equation in question into as 'simple' a form as possible. The normal form theory was extended to stochastic processes, with the main focus on bifurcation problems [26–28]. Furthermore, mathematical techniques for random normal forms have been developed [29]. However, as far as we are aware, the transformation of (1) to (5) has never been presented.

In another related work, a generalized Langevin equation with a memory function was derived from a nonlinear Langevin equation by employing a projection operator method [19]. In this method, functions of dynamical variables are projected onto a subspace of interest, by using the so-called Mori identity [30]. Then, the choice of the projection operator represents the essence of the problem when considering whether the obtained result is physically meaningful, as pointed out in [31]. However, as far as we understand, there was no such discussion in [19]. Of course, whatever method we use, the important point is whether the obtained result is related to quantities and relations that can be measured experimentally. The determination of dissipative and other forces should be done in such a way that it is clear how they can be measured experimentally.

Acknowledgments

Appendix A. Verifying formula (57)

Here, we confirm the validity of formula (57) by directly calculating the response function from its definition (10). To this end, we utilize a perturbation force, $f_p(t)$, that takes the form of a step function: $f_p(t) = 0$ for $t \leqslant 0$ and $f_p(t) = 1$ for $t > 0$. Then, we have

$$\langle \dot{x}(t) \rangle_\varepsilon - v_s = \varepsilon \int_0^t ds\, R(s) + O(\varepsilon^2). \tag{A.1}$$

Using (3), the left-hand side of this equation can be expressed as

$$\langle \dot{x}(t) \rangle_\varepsilon - v_s = \int_0^\ell d\theta\, p_\infty(\theta, t) \frac{F(\theta) + \varepsilon f_p(t)}{\gamma} - v_s. \tag{A.2}$$

The function $p_\infty(\theta, t)$ satisfies the equation

$$\frac{\partial}{\partial t} p_\infty(\theta, t) = \left(\mathcal{L}_{FP} - \frac{\varepsilon}{\gamma} f_p(t) \frac{\partial}{\partial \theta} \right) p_\infty(\theta, t), \tag{A.3}$$

with the initial condition $p_\infty(\theta, 0) = p_{st}(\theta)$.

Substituting the expanded form (4) into (A.3) and extracting terms proportional to ε, we obtain

$$\frac{\partial}{\partial t} p^{(1)}(\theta, t) = \mathcal{L}_{FP} p^{(1)}(\theta, t) - \frac{1}{\gamma} f_p(t) p'_{st}(\theta). \tag{A.4}$$

Next, we write $p^{(1)}(\theta, t)$ in terms of the eigenfunctions of $\mathcal{L}_{FP}$:

$$p^{(1)}(\theta, t) = \sum_{j=-\infty}^{\infty} p_j^{(1)}(t) \Psi_j^*(\theta). \tag{A.5}$$

Substituting this form into (A.4), we obtain

$$\dot{p}_j^{(1)}(t) = -\lambda_j p_j^{(1)}(t) + \frac{1}{\gamma} f_p(t) (\Psi_0, \Phi'_j). \tag{A.6}$$

Integration of (A.6) with the initial condition $p_j^{(1)}(0) = 0$ yields

$$p_j^{(1)}(t) = \frac{1}{\gamma} f_p(t) (\Psi_0, \Phi'_j) \int_0^t ds\, e^{-\lambda_j s}. \tag{A.7}$$

Using the results (A.5) and (A.7), we express (A.2) as

$$\langle \dot{x}(t) \rangle_\varepsilon - v_s = \frac{\varepsilon}{\gamma} \left[f_p(t) + \frac{1}{\gamma} \sum_{j=-\infty}^{\infty} f_p(t)(\Psi_0, \Phi_j')(\Psi_j, F) \int_0^t ds\, e^{-\lambda_j s} \right] + O(\varepsilon^2). \tag{A.8}$$

Comparing this with (A.1), we find

$$\gamma R(t) = \delta(t) + \sum_{j=-\infty}^{\infty} \frac{1}{\gamma}(\Psi_j, F)\, e^{-\lambda_j t}(\Psi_0, \Phi_j'). \tag{A.9}$$

The Fourier transformation of this relation gives

$$\gamma \tilde{R}(\omega) = 1 + \sum_{j=-\infty}^{\infty} \frac{1}{\gamma} \frac{(\Psi_j, F)}{\lambda_j - i\omega}(\Psi_0, \Phi_j'), \tag{A.10}$$

which is found to be equivalent to (62).

Appendix B. Proof of (69)

Differentiating (33) with respect to θ, we obtain

$$\Lambda^\ddagger \Phi_j' = -\lambda_j \Phi_j', \tag{B.1}$$

with

$$\Lambda^\ddagger \equiv -\frac{1}{\gamma} \frac{\partial}{\partial \theta} V'(\theta) + \frac{T}{\gamma} \frac{\partial^2}{\partial \theta^2}. \tag{B.2}$$

Because Φ_j' is an eigenfunction of $\Lambda^\ddagger$, below we employ the notation

$$\Phi_j^\ddagger \equiv \Phi_j'. \tag{B.3}$$

The operator adjoint to $\Lambda^\ddagger$, $\mathcal{L}_{FP}^\ddagger$ is defined through the following:

$$\left(\mathcal{L}_{FP}^\ddagger h_1, h_2 \right) \equiv (h_1, \Lambda^\ddagger h_2). \tag{B.4}$$

The explicit form of $\mathcal{L}_{FP}^\ddagger$ is

$$\mathcal{L}_{FP}^\ddagger = \frac{1}{\gamma} V'(\theta) \frac{\partial}{\partial \theta} + \frac{T}{\gamma} \frac{\partial^2}{\partial \theta^2}. \tag{B.5}$$

The set of eigenvalues, $-\lambda_j$, of this operator $\mathcal{L}_{FP}^\ddagger$ is identical to that of $\Lambda^\ddagger$. The corresponding eigenfunctions $\Psi_j^\ddagger$ are labelled such that they satisfy the equation

$$\mathcal{L}_{FP}^\ddagger \Psi_j^\ddagger = -\lambda_j^* \Psi_j^\ddagger. \tag{B.6}$$

These eigenfunctions can be chosen so as to satisfy the orthogonality condition

$$\left(\Psi_i^\ddagger, \Phi_j^\ddagger \right) = \delta_{ij}. \tag{B.7}$$

Then, differentiating (B.6) with respect to θ, we obtain

$$\mathcal{L}_{FP} \Psi_j^{\ddagger\prime} = -\lambda_j^* \Psi_j^{\ddagger\prime}. \tag{B.8}$$

Thus, applying (B.7), we have

$$\Psi_j^{\ddagger\prime} = -\Psi_j \tag{B.9}$$

for the case $j \neq 0$, and $\Psi_0^\ddagger = 1$.

Now, we define the quantity $Q(\theta)$ as

$$Q(\theta) \equiv -\frac{1}{\gamma} \sum_{j=-\infty}^{\infty} \frac{(\Psi_j, V')}{\lambda_j} \Phi'_j(\theta). \tag{B.10}$$

Using (B.3), we calculate

$$\Lambda^{\ddagger} Q = \frac{1}{\gamma} V''. \tag{B.11}$$

Solving this equation, we obtain

$$Q(\theta) = -1 + q_1 e^{\beta V(\theta)} \int_0^\theta d\theta' \, e^{-\beta V(\theta')} + q_2 e^{\beta V(\theta)}. \tag{B.12}$$

The two constants q_1 and q_2 here are determined by the conditions

$$Q(0) = Q(\ell), \tag{B.13}$$

$$\left(\Psi_0^{\ddagger}, Q\right) = 0. \tag{B.14}$$

Condition (B.13) leads to

$$q_2 = q_1 \frac{1}{e^{\beta f \ell} - 1} \int_0^\ell d\theta' \, e^{-\beta V(\theta')}. \tag{B.15}$$

Substituting this into (B.12), we obtain

$$1 + Q(\theta) = q_1 \frac{e^{\beta V(\theta)}}{e^{\beta f \ell} - 1} \left[\int_0^\ell d\theta' \, e^{-\beta V(\theta')} - (1 - e^{\beta f \ell}) \int_0^\theta d\theta' \, e^{-\beta V(\theta')} \right]$$

$$= \frac{q_1}{e^{\beta f \ell} - 1} I_+(\theta), \tag{B.16}$$

where we have used identity (67). Using (B.16) in (B.14) leads to the final form (69).

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