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2006 J. Phys. A: Math. Gen. 39 8593

(http://iopscience.iop.org/0305-4470/39/27/003)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **39** (2006) 8593–8601 doi:10.1088/0305-4470/39/27/003

Existence and construction of dynamical potential in nonequilibrium processes without detailed balance

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Received 21 November 2005, in final form 27 April 2006
Published 21 June 2006
Online at stacks.iop.org/JPhysA/39/8593

Abstract

The existence of a dynamical potential with both local and global meanings in general nonequilibrium processes has been controversial. Following an earlier heuristic argument in a letter by one of us, in the present paper we show rigorously its existence for a generic class of situations in physical and biological sciences. The local dynamical meaning of this potential function is demonstrated via a special stochastic differential equation and its global steady-state meaning via a novel and explicit form of the Fokker–Planck equation. We also give a procedure to obtain the special stochastic differential equation for any given Fokker–Planck equation. No detailed balance condition is required in our demonstration. For the first time we obtain here a formula to describe the noise-induced shift in drift force compared to the steady-state distribution, a phenomenon extensively observed in numerical studies.

PACS numbers: 05.10.Gg, 72.70.+m

1. Formulation of the questions

A large class of nonequilibrium processes can be described by the following stochastic differential equation [1–4]:

$$\dot{\mathbf{q}} = \mathbf{f}(\mathbf{q}) + N_I(\mathbf{q})\xi(t), \tag{1}$$

where $\mathbf{f}$ and $\mathbf{q}$ are n-dimensional vectors and $\mathbf{f}$ a nonlinear function of $\mathbf{q}$. The noise ξ is a standard Gaussian white noise with l independent components: $\langle\xi_i\rangle = 0$, $\langle\xi_i(t)\xi_j(t')\rangle = \delta_{ij}\delta(t-t')$ and $i, j = 1, 2, \ldots, l$. Even in situations that equation (1) is not an exact description, it may still serve as the first approximation for further modelling [3, 4].

A further description of the noise in equation (1) is through the $n \times n$ diffusion matrix $D(\mathbf{q})$, which is defined by the following matrix equation:

$$N_I(\mathbf{q})N_I^\tau(\mathbf{q}) = 2\epsilon D(\mathbf{q}), \tag{2}$$

where N_I is an $n \times l$ matrix, N_I^τ is its transpose and ϵ is a non-negative numerical constant playing the role of temperature. This relation suggests that the $n \times n$ diffusion matrix D is both symmetric and non-negative. For the dynamics of state vector $\mathbf{q}$, all that is needed from the noise is the diffusion matrix D. Hence, it is not necessary to require the dimension of the noise vector ξ to be the same as that of the state vector $\mathbf{q}$. This implies that in general $l \neq n$. The difficulty for finding such a potential function can be illustrated by the fact that usually $D^{-1}(\mathbf{q})\mathbf{f}(\mathbf{q})$ cannot be written as a gradient of the scalar function [1, 3] when no detailed balance condition is assumed in equation (1). Here and below, without loss of generality the functions, such as $\mathbf{f}(\mathbf{q})$ and $D(\mathbf{q})$, are assumed to be sufficiently smooth. The boundary conditions will be chosen accordingly. This means that boundary conditions such as absorbing type will not be considered here, though they can be treated as appropriate limits of the smooth functions.

During the study of the robustness of the genetic switch in a living organism [5], it was discovered that equation (1) can be transformed into the following form:

$$[S(\mathbf{q}) + T(\mathbf{q})]\dot{\mathbf{q}} = -\nabla_{\mathbf{q}}\phi(\mathbf{q}) + N_{II}(\mathbf{q})\xi(t), \tag{3}$$

where the noise ξ is from the same source as that in equation (1). The $n \times n$ matrices are the symmetric non-negative friction matrix S and the antisymmetric matrix T, and

$$S(\mathbf{q}) + T(\mathbf{q}) = \frac{1}{[D(\mathbf{q}) + Q(\mathbf{q})]} \equiv M(\mathbf{q}). \tag{4}$$

Here Q is an antisymmetric matrix determined by both the diffusion matrix $D(\mathbf{q})$ and the deterministic force $\mathbf{f}(\mathbf{q})$ [6, 7]. The potential function $\phi(\mathbf{q})$ is connected to the deterministic force $\mathbf{f}(\mathbf{q})$ by

$$\nabla_{\mathbf{q}}\phi(\mathbf{q}) = -M(\mathbf{q})\mathbf{f}(\mathbf{q}). \tag{5}$$

The friction matrix $S(\mathbf{q})$ is defined through the following matrix equation:

$$N_{II}(\mathbf{q})N_{II}^\tau(\mathbf{q}) = 2\epsilon S(\mathbf{q}), \tag{6}$$

which guarantees that S is both symmetric and non-negative. For simplicity, we will assume $\det(S) \neq 0$ in the rest of the paper. It is a sufficient condition for $\det(M) \neq 0$ and more general cases are also known [6]. The breakdown of the detailed balance condition or the time-reversal symmetry is represented by the finiteness of the transverse matrix T. The usefulness of this formulation is already manifested in the successful solution of outstanding stability puzzle along with new predictions in gene regulatory dynamics [5].

It was heuristically argued by one of us [7] that the global steady-state distribution $\rho(\mathbf{q})$ in the state space is, if it exists,

$$\rho(\mathbf{q}) \propto \exp\left(-\frac{\phi(\mathbf{q})}{\epsilon}\right). \tag{7}$$

By construction the fixed points of the deterministic force $\mathbf{f}$ in equation (1) are also the extremal points of the potential function ϕ in equation (3) and (7). Therefore, the potential function ϕ acquires both the local dynamical meaning through equation (3) and the global steady-state meaning through equation (7). This heuristical demonstration has been rigorously shown to be locally valid for any fixed point, stable or unstable [6]. Two major questions, however, remain unanswered: can the heuristical argument be translated into an explicit procedure such that there is an explicit Fokker–Planck equation whose steady-state solution is indeed given by equation (7)? Is the converse also true, that is, for a given Fokker–Planck equation, can the corresponding equation (3) be found? Furthermore, are there new and significant results? In this paper we give affirmative answers to all those important questions: the general stage is set in section 2; The answer to the first question is given in section 3; the awswer to the converse question is given in section 4, and new and significant results are discussed in sections 3–5.

2. Derivation of a generalized Klein–Kramers equation

Central in the heuristical argument is the introduction of an n-dimensional kinetic momentum $\mathbf{p}$ along with a mass m. This procedure brings the stochastic differential equations in close contact with the Hamiltonian or symplectic structure central in theoretical physics. The mass would eventually be taken to be zero to recover equation (3). The dynamical equation for the enlarged state space is now $2n$ dimensions and the extended stochastic dynamical equation takes the form [7]

$$\dot{\mathbf{q}} = \frac{\mathbf{p}}{m}, \qquad \dot{\mathbf{p}} = -M(\mathbf{q})\frac{\mathbf{p}}{m} - \nabla_{\mathbf{q}}\phi(\mathbf{q}) + N_{II}(\mathbf{q})\xi(t), \tag{8}$$

which is in the form of the standard Langevin physics in the $(\mathbf{p}, \mathbf{q})$ phase space. A similar equation has been extensively studied in the literature [3, 4]. Here, we investigate it from a different perspective, the zero-mass limit.

To proceed, we first give an independent derivation of the generalized Fokker–Planck equation, the so-called Klein–Kramers equation [3] in a general form, corresponding to equation (8). We will show that there is no ambiguity in the treatments of stochastic differential equation at this stage. The probability distribution function in the $(\mathbf{p}, \mathbf{q})$ phase space is defined by

$$\rho(\mathbf{p}, \mathbf{q}, t) \equiv \langle \delta(\mathbf{p} - \bar{\mathbf{p}}(t, \{\xi\}))\delta(\mathbf{q} - \bar{\mathbf{q}}(t, \{\xi\}))\rangle, \tag{9}$$

where $\bar{\mathbf{q}}(t, \{\xi\})$ and $\bar{\mathbf{p}}(t, \{\xi\})$ are the solution of equation (8) for a given noise configuration $\{\xi\}$. The distribution function ρ is obtained by averaging over all the noise configurations, which is an ensemble average.

With variables $(\bar{\mathbf{q}}(t), \bar{\mathbf{p}}(t))$ following equation (8), the time derivative of the distribution function ρ is given by

$$\partial_t \rho(\mathbf{p}, \mathbf{q}, t) = \nabla_{\mathbf{p}} \cdot \left[M(\mathbf{q})\frac{\mathbf{p}}{m} + \nabla_{\mathbf{q}}\phi(\mathbf{q}) \right] \rho(\mathbf{p}, \mathbf{q}, t) - \nabla_{\mathbf{q}} \cdot \frac{\mathbf{p}}{m}\rho(\mathbf{p}, \mathbf{q}, t)$$
$$- \nabla_{\mathbf{p}} \cdot N_{II}(\mathbf{q})\langle \xi(t)\delta(\mathbf{q} - \bar{\mathbf{q}})\delta(\mathbf{p} - \bar{\mathbf{p}})\rangle. \tag{10}$$

Using an identity due to Novikov [8],

$$\langle \xi(t) g[\{\xi\}]\rangle = \langle \delta g[\{\xi\}]/\delta\xi(t)\rangle\,, \tag{11}$$

where g is a functional of the noise $\{\xi\}$, and using the convention

$$\delta \left[\int_0^t \xi(t')\, \mathrm{d}t \right] \Big/ \delta\xi(t) = 1/2, \tag{12}$$

and noting that the solution of equation (8) can be formally expressed as

$$\bar{\mathbf{q}}(t) - \mathbf{q}(0) = \int_0^t \bar{\mathbf{p}}\, \mathrm{d}t'/m \tag{13}$$

$$\bar{\mathbf{p}}(t) - \mathbf{p}(0) = -\int_0^t [M(\bar{\mathbf{q}})\bar{\mathbf{p}}/m - \nabla_{\bar{\mathbf{q}}}\phi(\bar{\mathbf{q}}) + N_{II}(\bar{\mathbf{q}})\xi]\, \mathrm{d}t', \tag{14}$$

we have the following relations:

$$\delta\bar{\mathbf{q}}(t)/\delta\xi(t) = 0, \tag{15}$$

$$\delta\bar{\mathbf{p}}(t)/\delta\xi(t) = N_{II}^{\tau}(\bar{\mathbf{q}})/2. \tag{16}$$

The last term on the right-hand side of equation (10) is thus given by

$$-\nabla_{\mathbf{p}} \cdot N_{II}(\mathbf{q})\langle \xi(t)\delta(\mathbf{q} - \bar{\mathbf{q}})\delta(\mathbf{p} - \bar{\mathbf{p}})\rangle = \nabla_{\mathbf{p}} \cdot N_{II}(\mathbf{q})\tfrac{1}{2}N_{II}^{\tau}(\mathbf{q})\nabla_{\mathbf{p}}\rho(\mathbf{p}, \mathbf{q}, t), \tag{17}$$

Combining equations (10) and (17), we obtain the Klein–Kramers equation, a special form of the Fokker–Planck equation,

$$\partial_t \rho(\mathbf{p}, \mathbf{q}, t) = \nabla_{\mathbf{p}} \cdot \left[M(\mathbf{q}) \frac{\mathbf{p}}{m} + \nabla_{\mathbf{q}} \phi(\mathbf{q}) + \epsilon S(\mathbf{q}) \nabla_{\mathbf{p}} \right] \rho(\mathbf{p}, \mathbf{q}, t) - \nabla_{\mathbf{q}} \cdot \frac{\mathbf{p}}{m} \rho(\mathbf{p}, \mathbf{q}, t). \tag{18}$$

A special case of equation (18) has been known [3]. Here we have generalized it to any allowed matrix M. It has the stationary solution, if it exists,

$$\rho(\mathbf{p}, \mathbf{q}) = \exp\left(- \frac{\left[\frac{p^2}{2m} + \phi(\mathbf{q}) \right]}{\epsilon} \right), \tag{19}$$

which holds for all possible values of mass m.

We should point out that starting from equation (8) same equation (18) can be arrived by either Ito or Stratonovich prescription of stochastic integration, because $\nabla_{\mathbf{p}}^{\tau} M(\mathbf{q}) = 0$. Equation (19) has been used in the heuristic demonstration [7], to make use of its insensitivity to various treatments of stochastic differential equation.

3. Zero-mass limit and the desired Fokker–Planck equation

Now we are ready to take the zero-mass limit and to derive the Fokker–Planck equation corresponding to equation (3). We first define following two operators:

$$L_1 \equiv \nabla_{\mathbf{p}}^{\tau} M(\mathbf{q}) \left[\epsilon \nabla_{\mathbf{p}} + \frac{\mathbf{p}}{m} \right], \tag{20}$$

$$L_2 \equiv -\frac{\mathbf{p}}{m} \cdot \nabla_{\mathbf{q}} + \nabla_{\mathbf{q}} \phi(\mathbf{q}) \cdot \nabla_{\mathbf{p}}. \tag{21}$$

With those two operators, equation (18) becomes

$$\partial_t \rho(\mathbf{p}, \mathbf{q}, t) = (L_1 + L_2) \rho(\mathbf{p}, \mathbf{q}, t). \tag{22}$$

The antisymmetric properties $\nabla_{\mathbf{p}}^{\tau} T(\mathbf{q}) \nabla_{\mathbf{p}} = 0$ and $\mathbf{p}^{\tau} T(\mathbf{q}) \mathbf{p} = 0$ are used in the above equation.

There are various ways to eliminate the fast degrees of freedom of $\mathbf{q}$ implied in the zero-mass limit, such as the dynamical renormalization method [9] and the projection operator method [4, 10, 11]. In the following, we adopt from Gardiner [4] the standard projection operator method for its conciseness. For further exposition of this method, we refer readers to [10, 11].

Following Gardiner, we introduce a projection operator

$$P h(\mathbf{p}, \mathbf{q}, t) \equiv \frac{1}{(2\pi m \epsilon)^{n/2}} \exp\left(-\frac{p^2}{2m\epsilon} \right) \int h(\mathbf{p}', \mathbf{q}, t) \, \mathrm{d}^n p', \tag{23}$$

where h is an arbitrary function of $\mathbf{p}$, $\mathbf{q}$.

The eigenvalues of the projection operator can only be zero or one,

$$P^2 = P, \tag{24}$$

which follows from the relation

$$\begin{aligned} P^2 h(\mathbf{p}, \mathbf{q}, t) &= \frac{1}{(2\pi m \epsilon)^{n/2}} \exp\left(-\frac{p^2}{2m\epsilon} \right) \int \frac{\mathrm{d}^n p_1}{(2\pi m \epsilon)^{n/2}} \exp\left(-\frac{p_1^2}{2m\epsilon} \right) \int h(\mathbf{p}_2, \mathbf{q}, t) \, \mathrm{d}^n p_2 \\ &= \frac{1}{(2\pi m \epsilon)^{n/2}} \exp\left(-\frac{p^2}{2m\epsilon} \right) \int h(\mathbf{p}', \mathbf{q}, t) \, \mathrm{d}^n p' \\ &= P h(\mathbf{p}, \mathbf{q}, t). \end{aligned} \tag{25}$$

From the fact

$$\left(\epsilon\nabla_{\mathbf{p}} + \frac{\mathbf{p}}{m}\right)\exp\left(-\frac{p^2}{2m\epsilon}\right) = 0, \tag{26}$$

we obtain the identity

$$L_1 P = 0. \tag{27}$$

Since L_1 is a total derivative operator, for any function $h(\mathbf{p}, \mathbf{q}, t)$ that is well behaved at the boundary (infinity), the function $PL_1h(\mathbf{p}, \mathbf{q}, t)$ vanishes, because

$$\begin{aligned} PL_1h(\mathbf{p}, \mathbf{q}, t) &= \frac{1}{(2\pi m\epsilon)^{n/2}}\exp\left(-\frac{p^2}{2m\epsilon}\right)\int \nabla^{\tau}_{\mathbf{p}'}M(\mathbf{q})\left[\epsilon\nabla_{\mathbf{p}'} + \frac{\mathbf{p}'}{m}\right]h(\mathbf{p}', \mathbf{q}, t)\,\mathrm{d}^n p' \\ &= \frac{1}{(2\pi m\epsilon)^{n/2}}\exp\left(-\frac{p^2}{2m\epsilon}\right)\oint_{\mathrm{B.C.}} \mathrm{d}\mathbf{S}\cdot\nabla^{\tau}_{\mathbf{p}'}M(\mathbf{q})\left[\epsilon\nabla_{\mathbf{p}'} + \frac{\mathbf{p}'}{m}\right]h(\mathbf{p}', \mathbf{q}, t) \\ &= 0, \end{aligned}$$

where $\mathrm{d}\mathbf{S}$ is the surface element with direction. From the last two identities, we can see that the operator L_1 is orthogonal to the projection operator P. We further have $PL_2P = 0$, due to the inversion symmetry in the $\mathbf{p}$-space,

$$\int \frac{\mathrm{d}^n p}{(2\pi m\epsilon)^{n/2}}\left[-\frac{\mathbf{p}}{m}\cdot\nabla_{\mathbf{q}} + \nabla_{\mathbf{q}}\phi(\mathbf{q})\cdot\nabla_{\mathbf{p}}\right]\exp\left(-\frac{p^2}{2m\epsilon}\right) = 0. \tag{28}$$

To proceed, we first separate the distribution function into the projected part $v(\mathbf{p}, \mathbf{q}, t) \equiv P\rho(\mathbf{p}, \mathbf{q}, t)$ and unprojected part $w(\mathbf{p}, \mathbf{q}, t) \equiv (1-P)\rho(\mathbf{p}, \mathbf{q}, t)$. We further define the reduced distribution function $\rho(\mathbf{q}, t)$ through the projected part:

$$v(\mathbf{p}, \mathbf{q}, t) \equiv \frac{1}{(2\pi m\epsilon)^{n/2}}\exp\left(-\frac{p^2}{2m\epsilon}\right)\rho(\mathbf{q}, t). \tag{29}$$

The dynamical equations for v and w can be obtained separately from equation (22)

$$\partial_t v = P\partial_t\rho = P(L_1 + L_2)(v + w) = PL_2 w, \tag{30}$$

$$\partial_t w = \partial_t\rho - P\partial_t\rho = (L_1 + L_2)w + L_2 v - PL_2 w. \tag{31}$$

After the Laplace transformation $\tilde{h}(s) = \int_0^\infty h(t)\exp(-st)\,\mathrm{d}t$, these two equations take the form $\tilde{v} - v(0) = PL_2\tilde{w}$ and $s\tilde{w} - w(0) = (L_1 + L_2)\tilde{w} + L_2\tilde{v} - PL_2\tilde{w}$. The latter expression is equivalent to

$$\tilde{w} = [s - L_1 - (1 - P)L_2]^{-1}[L_2\tilde{v} + w(0)]. \tag{32}$$

We note that following equation (8) the relaxation time for $\mathbf{p}$ dynamics is of the order of m. In the zero-mass limit, this relaxation time is very short. After sufficiently long time, that is, $t \gg m$, which is still short comparing to the dynamics of the $\mathbf{q}$, the momentum distribution is essentially described by the white noise and its fluctuation range is of the order of $\sqrt{m}$. Its mean distribution would be determined by the slow dynamics of $\mathbf{q}$. Therefore, we are looking for the low-frequency behaviour of the transformed equation: the leading contribution when $s \ll 1/m$. At low frequency, to the leading order of m, the momentum $\mathbf{p}$ scales with $\sqrt{m}$, L_1 is of the order of $1/m$ and L_2 is of the order of $1/\sqrt{m}$. Hence, at low frequency to the leading contribution ordered by m, equation (32) leads to

$$\tilde{w} = -L_1^{-1}L_2\tilde{v} + O(m), \tag{33}$$

which is a precise statement on the adiabatic following the kinetic momentum $\mathbf{p}$ to the coordinate $\mathbf{q}$. The equation for v is thus given by

$$\partial_t v = -PL_2L_1^{-1}L_2 v + O(\sqrt{m}). \tag{34}$$

We recall an identity to be used. The operator L_1 has a null space and its inverse operator is not well defined unless in the space orthogonal to the null space. For an arbitrary vector $\mathbf{c}(\mathbf{q})$ which has no $\mathbf{p}$-dependence, the following identity holds:

$$L_1 \mathbf{p} \cdot \mathbf{c}(\mathbf{q}) \exp\left(-\frac{p^2}{2m\epsilon}\right) = \epsilon \nabla_{\mathbf{p}} \cdot M(\mathbf{q})\mathbf{c}(\mathbf{q}) \exp\left(-\frac{p^2}{2m\epsilon}\right) = -\frac{\mathbf{p}}{m} \cdot M(\mathbf{q})\mathbf{c}(\mathbf{q}) \exp\left(-\frac{p^2}{2m\epsilon}\right). \quad (35)$$

We note that $L_2 v$ takes the form of the right-hand side of equation (35), and is therefore orthogonal to the null space of L_1. The inverse operator L_1^{-1} is then well defined. Using the inverse relation of equation (35) we arrive at the desired identity:

$$L_1^{-1} \frac{\mathbf{p}}{m} \cdot \mathbf{c}(\mathbf{q}) \exp\left(-\frac{p^2}{2m\epsilon}\right) = -\mathbf{p} \cdot M^{-1}(\mathbf{q})\mathbf{c}(\mathbf{q}) \exp\left(-\frac{p^2}{2m\epsilon}\right). \quad (36)$$

With the above identity, the right-hand side of equation (34) is given by

$$-PL_2L_1^{-1}L_2 v = PL_2L_1^{-1}\frac{\mathbf{p}}{m} \cdot \left[\nabla_{\mathbf{q}} + \frac{1}{\epsilon}\nabla_{\mathbf{q}}\phi(\mathbf{q})\right] v = \nabla_{\mathbf{q}} \cdot M^{-1}(\mathbf{q})[\epsilon\nabla_{\mathbf{q}} + \nabla_{\mathbf{q}}\phi(\mathbf{q})]v. \quad (37)$$

Therefore in the zero-mass limit, $m \to 0$, the equation for the integrated probability distribution $\rho(\mathbf{q}, t)$ defined in equation (29) takes the form, as a direct consequence of equation (34) and (37),

$$\partial_t \rho(\mathbf{q}, t) = \nabla_{\mathbf{q}} M^{-1}(\mathbf{q})[\epsilon\nabla_{\mathbf{q}} + \nabla_{\mathbf{q}}\phi(\mathbf{q})]\rho(\mathbf{q}, t). \quad (38)$$

This is the sought Fokker–Planck equation corresponding to equation (3). We point out that in the above derivation we take the mass to be zero, keeping other parameters, including the friction and transverse matrices, finite. On the other hand, in the usual Smoluchowski limit it is the friction matrix that has to be taken as infinite, keep all other parameters finite. Those two limits are in general not interchangeable.

The equilibrium configuration solution of equation (38) is the same as equation (7). Again, we emphasize that no detailed balance condition is assumed in reaching this result. This completes our answer to the first question of finding the corresponding Fokker–Planck equation.

4. Converse problem

We now address the second main question that for any given Fokker–Planck equation there is the corresponding stochastic differential equation, i.e. equation (3). We will give an affirmative answer, which closes a logic gap in the light of present formulation. The procedure to carry it out is already implicitly contained in equation (38), a typical situation in theoretical physics that if the answer is known a procedure to obtain it can be easily found. In addition, the demonstration in this section also supplements above rather abstract projection operator demonstration.

A generic Fokker–Planck equation for the dynamics of probability density in state space may take the form

$$\partial_t \rho(\mathbf{q}, t) = \nabla_{\mathbf{q}}^{\tau}[\epsilon \overline{D}(\mathbf{q})\nabla_{\mathbf{q}} - \overline{\mathbf{f}}(\mathbf{q})]\rho(\mathbf{q}, t). \quad (39)$$

Here $\overline{D}(\mathbf{q})$ is the diffusion matrix and $\overline{\mathbf{f}}(\mathbf{q})$ is the drift force. A potential function $\overline{\phi}(\mathbf{q})$ can always be defined from the steady-state distribution. This has been extensively studied in mathematics [12]. Given the existence of the potential function, the procedure is particularly simple.

Using $M^{-1}(\mathbf{q}) = D(\mathbf{q}) + Q(\mathbf{q})$ [7], equation (38) can be rewritten as

$$\partial_t \rho(\mathbf{q}, t) = \nabla_{\mathbf{q}}^{\tau}\left[\epsilon D(\mathbf{q})\nabla_{\mathbf{q}} - \epsilon\left(\nabla_{\mathbf{q}}^{\tau} Q(\mathbf{q})\right)^{\tau} + [D(\mathbf{q}) + Q(\mathbf{q})]\nabla_{\mathbf{q}}\phi(\mathbf{q})\right]\rho(\mathbf{q}, t). \tag{40}$$

The antisymmetric property of the matrix $Q(\mathbf{q})$ has been used in reaching equation (40). Thus, comparing between equation (39) and (40), we have $D(\mathbf{q}) = \overline{D}(\mathbf{q})$, $\phi(\mathbf{q}) = \overline{\phi}(\mathbf{q})$, and

$$\mathbf{f}(\mathbf{q}) = \bar{\mathbf{f}}(\mathbf{q}) - \epsilon\left(\nabla_{\mathbf{q}}^{\tau} Q(\mathbf{q})\right)^{\tau}. \tag{41}$$

In reaching equation (41) we have used the relation $[D(\mathbf{q}) + Q(\mathbf{q})]\nabla_{\mathbf{q}}\phi(\mathbf{q}) = -\mathbf{f}(\mathbf{q})$. The explicit equation for the antisymmetric matrix Q is

$$-\epsilon\left(\nabla_{\mathbf{q}}^{\tau} Q(\mathbf{q})\right)^{\tau} + [D(\mathbf{q}) + Q(\mathbf{q})]\nabla_{\mathbf{q}}\phi(\mathbf{q}) = -\bar{\mathbf{f}}(\mathbf{q}). \tag{42}$$

The solution for Q can be formally written as

$$Q(\mathbf{q}) = -\frac{1}{\epsilon}\int^{\mathbf{q}} \mathrm{d}\mathbf{q}'[\bar{\mathbf{f}}(\mathbf{q}') + D(\mathbf{q}')\nabla_{\mathbf{q}'}\phi(\mathbf{q}')]\exp\left(\frac{\phi(\mathbf{q}') - \phi(\mathbf{q})}{\epsilon}\right) + Q_0(\mathbf{q})\exp\left(-\frac{\phi(\mathbf{q})}{\epsilon}\right). \tag{43}$$

Here $Q_0(\mathbf{q})$ is a solution of the homogeneous equation $\epsilon\nabla_{\mathbf{q}}^{\tau} Q(\mathbf{q}) = 0$, and the two parallel vectors in the integrand, such as $\mathrm{d}\mathbf{q}'\,\bar{\mathbf{f}}(\mathbf{q})$, form a matrix. This completes our answer to the converse question of finding the corresponding stochastic differential equation in the form of equation (3) from any given Fokker–Planck equation.

We note that the shift between the zeros of the potential gradient and the drift force is given by, from equation (41),

$$\Delta\bar{\mathbf{f}} = -\epsilon\left(\nabla_{\mathbf{q}}^{\tau} Q(\mathbf{q})\right)^{\tau}, \tag{44}$$

that is, the extremals of the steady-state distribution are not necessarily determined by the zeros of drift force $\bar{\mathbf{f}}$. To our knowledge this is the first time that such an analytic formula for the shift is obtained.

It is worthwhile to point out that a construction similar to that of above was discussed in [13]. In order to obtain the desired potential function, several additional conditions, including one similar to set $\nabla_{\mathbf{q}} Q(\mathbf{q}) = 0$ (4.18), were required in [13]. Our present demonstration shows that there is no need for those conditions. Hence, our construction may be regarded as a generalization of the corresponding one in [13].

5. Discussions

Attempts to decompose the dynamics into the dissipative and transverse parts were extensively explored in the literature in the framework of Fokker–Planck equation [14, 15]. Though conceptually the basic ideas in the literature are similar to what discussed here, the present demonstration shows that in general there is no apparent separation between the friction and the transverse matrices implied in those previous works, because the gradient of the antisymmetric matrix Q in equation (41) is in general not zero. The antisymmetric matrix Q should be determined by both diffusion matrix D and deterministic force $\mathbf{f}$ in equation (1) or by both friction and transverse matrices in equation (3). Furthermore, the connection between the local micro-dynamics describing by equation (3) and the global macro-dynamics discussed in equation (41), or equation (42) or (43), was not discussed in [14, 15]. In fact, the present authors were not aware of such a connection prior to 2004 [6, 7]. We should remark here that the special form of the stochastic differential equation, i.e. equation (3), is consistent with the formulation of dissipative dynamics from first principles [10, 16].

If the antisymmetric matrix Q is zero, there would be no shift between the zeros of drift force and the potential gradient according to equations (38) and (39). The drift force in this case can be expressed as $\bar{\mathbf{f}}(\mathbf{q}) = -D(\mathbf{q})\nabla_{\mathbf{q}}\phi(\mathbf{q})$, exactly the detailed balance condition. However, even if D is independent of the state vector, that is, there is no difference between Ito and Stratonovich treatments of stochastic differential equations, the antisymmetric matrix Q can still be state vector dependent. There would still be a shift between the zero of the potential gradient and the drift force. This is precisely what have been found in numerical studies on noise-induced phase transitions and bifurcations [17]. Equation (44) is a formula for this shift, which appears for the first time in the present paper.

There is an apparent disagreement between the singular behaviours found in the escape path study [18, 19] and a possible smooth potential function implied in the present study. While a detailed study on this feature is beyond the present paper, which will be reported elsewhere, we point out two main factors which are responsible for this apparent disagreement. The first factor is the difference in specifying the stochastic integration procedures. This difference results in a shift between the zeros of drift force and extremals of the steady-state distribution, described by the shift formula, equation (44). The second factor is that in [18] and [19] the focus is on the escaping rate and the corresponding escaping path, not on the steady-state distribution. The emergence of singularity is then not surprising, because its sensitivity to the dynamical elements, the transverse matrix T and the friction matrix S, in addition to the noise strength specified by ϵ.

Finally, there is another immediate and testable prediction from the present formulation. The limit cycle dynamics, abundant in nonequilibrium processes, has been used as a prototype example to argue against the existence of potential function. Not only our formulation suggests its existence in the sense of equations (3), (7) and (38), which is natural in theoretical physics, also it should take the same value along the limit cycle [20].

Acknowledgments

We thank critical and constructive discussions with D J Thouless, X-M Zhu, H Qian, C Kwon, M Dykman, Q Ouyang, R Mannella and P V E McClintock during the course of our investigation. We also thank G L Eyink for bringing our attention to [13] and for a following-up clarifying discussion. This work was supported in part by USA NIH grant under HG002894 and by China NSFC under grant number 90303008.

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