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Journal of Statistical Mechanics: Theory and Experiment
An IOP and SISSA journal

Beyond Itô versus Stratonovich

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Received 2 February 2012
Accepted 17 June 2012
Published 16 July 2012

Online at stacks.iop.org/JSTAT/2012/P07010
doi:10.1088/1742-5468/2012/07/P07010

Abstract. Recently, a novel framework to handle stochastic processes has emerged from a series of studies in biology, showing situations beyond 'Itô versus Stratonovich'. Its internal consistency can be demonstrated via the zero mass limit of a generalized Klein–Kramers equation. Moreover, the connection to other integrations becomes evident: the obtained Fokker–Planck equation defines a new type of stochastic calculus that in general differs from the α-type interpretation. A unique advantage of this new approach is a natural correspondence between stochastic and deterministic dynamics, which is useful or may even be essential in practice. The core of the framework is a transformation from the usual Langevin equation to a form that contains a potential function with two additional dynamical matrices, which reveals an underlying symplectic structure. The framework has a direct physical meaning and a straightforward experimental realization. A recent experiment has offered a first empirical validation of this new stochastic integration.

Keywords: Brownian motion, energy landscapes (theory), stochastic processes (theory), systems biology

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1742-5468/12/P07010+14$33.00

Contents

1. Introduction

The Itô–Stratonovich dilemma [1]–[3] on choosing the appropriate calculus when integrating stochastic differential equations (SDEs) has 'attracted considerable attention in the physics community' and 'is still as elusive as ever' [4]. Recent explorations of SDEs [5]–[16] have also been expanded into biology and other fields, generating new understanding on stochastic calculus. The novel framework [6], [9]–[11] in the present paper is *beyond* the Itô–Stratonovich controversy from two aspects. *First*, it defines a new type (named A-*type* for short) of stochastic integration that is different from Itô and Stratonovich's. In the one-dimensional case, A-type integration reduces to the α-type [4] with $\alpha = 1$ (Itô's corresponds to $\alpha = 0$ and Stratonovich's to $\alpha = 0.5$). In higher dimensional situations, it is generally not an α-type integration [16]. *Second*, there is a starting point in obtaining this new approach in which we need not choose the 'correct' calculus. One can reach the same result by the Itô, Stratonovich or A-type prescription of stochastic integration.

The effectiveness of the new framework has been demonstrated by various applications: successful solution of the outstanding stability puzzle of a genetic switch [5]; the quantification of the evolutionary dynamics of Darwin and Wallace [7]; the study of complex bio-networks such as metabolic networks [8] and cancer networks [12]; the implications of Darwinian dynamics in physics [13]; the relationship with Lyapunov's direct method for stability analysis in engineering [17]; the explicit construction of the adaptive landscape in population genetics [15], etc. Results of a recent experiment in

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one dimension [18] provide evidence that there exist processes in Nature choosing A-type integration.

A transformation from the classical Langevin equation to a structured form lies at the core of this framework. The significance of this transformation is the obtaining of a potential function that plays a dual role: it leads to the Boltzmann–Gibbs distribution on the final steady state (if it exists) of the stochastic process and it corresponds to the deterministic dynamics as a global Lyapunov function and can be used for stability analysis [17]. The potential function exists for general non-equilibrium processes without detailed balance [6, 10, 11], which have usually been difficult to handle by previous methods [19]. The behaviors near a fixed point, stable or not, have been exhaustively studied [9]; explicit construction for a simple limit cycle dynamics has been provided [20] as well. The structured form itself reveals the symplectic structure embedded in stochastic differential equations and has an invariant property [11] during the transformation. Other applications based on the concept of a potential function have also been studied in biology [14], [21]–[25], physics [26]–[28] and control theory [29, 30].

In the following, we first review the framework in section 2 with respect to the transformation and its consistency in mathematics. In section 3, several related issues are discussed, including a straightforward implication of the physical meaning. In particular, a one-dimensional experiment serving as an example is analyzed in section 3.3. We summarize in section 4.

2. The framework

A heuristic demonstration of this framework is given in section 2.1. It was first proposed by one of the authors in [6]. A more rigorous exposition [10] is then provided in section 2.2.

2.1. Review of the transformation

The stochastic differential equation, or the Langevin equation in physics, is usually a more precise description of reality than the purely deterministic one [1]–[3]. Additive noise is frequently considered for physical systems, but for biological or other complex systems a state variable dependent (multiplicative) noise is often encountered. In this paper we use the physicists' notation with a multiplicative noise

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

where $\mathbf{q}$, $\mathbf{f}$ are n-dimensional vectors and $\mathbf{f}$ is a nonlinear function of the state variable $\mathbf{q}$. The noise $\xi(t)$ is k-dimensional Gaussian white noise with zero mean, $\langle \xi(t) \rangle = 0$, and the covariance $\langle \xi(t)\xi^{\tau}(t') \rangle = \delta(t-t')I_k$. The superscript τ denotes the transpose of a matrix, $\delta(t-t')$ is the Dirac delta function, $\langle \cdots \rangle$ indicates the average over the noise distribution, I_k is the k-dimensional identity matrix. An element of the $n \times k$ matrix $N(\mathbf{q})$ can be a nonlinear function of $\mathbf{q}$. This matrix is further described by

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

where ϵ is a constant quantifying the noise strength and $D(\mathbf{q})$ is an $n \times n$ positive semi-definite diffusion matrix. Note that if the noise has less than n independent components, $k < n$, $D(\mathbf{q})$ has zero eigenvalue(s).

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During the study of a biological switch [5], a structured form equivalent to equation (1) was discovered,

$$[S(\mathbf{q}) + A(\mathbf{q})]\dot{\mathbf{q}} = -\nabla\phi(\mathbf{q}) + \hat{N}(\mathbf{q})\xi(t), \tag{3}$$

where $S(\mathbf{q})$ is symmetric and positive semi-definite, $A(\mathbf{q})$ is antisymmetric, $\phi(\mathbf{q})$ is the potential function, $\xi(t)$ is identical to that in equation (1) and the matrix $\hat{N}(\mathbf{q})$ is constrained by (see also section 3.1)

$$\hat{N}(\mathbf{q})\hat{N}^{\tau}(\mathbf{q}) = 2\epsilon S(\mathbf{q}). \tag{4}$$

We note that when $S = 0$, equation (3) has the same structure as the Hamiltonian equation in physics. The $(n = 2l)$-dimensional system (l generalized coordinates and l generalized momenta are combined in the n-dimensional system) with

$$A = \begin{pmatrix} 0 & I_l \\ -I_l & 0 \end{pmatrix}$$

and $\phi = H$ (the Hamiltonian) shows the embedded symplectic structure.

Two assumptions are implied in this framework. The *first* one is the equivalence of equations (1) and (3), that is, they are describing the same dynamical process. It is straightforward to go from equation (3) to equation (1), once $[S(\mathbf{q}) + A(\mathbf{q})]$ is nonsingular, which holds when the components q_i $(i = 1, \ldots, n)$ of the state variable $\mathbf{q} = (q_1, \ldots, q_n)^{\tau}$ are independent. The reverse, however, is much more difficult, including the need to obtain $S(\mathbf{q})$, $A(\mathbf{q})$ and $\phi(\mathbf{q})$ for general dynamics. Nevertheless, we can still assume, without a rigorous mathematical proof but rigorous enough from a working scientist's view, that the reverse part holds based on a case by case construction, that is, considering it as a protocol and not a theorem. Hence, we may replace $\dot{\mathbf{q}}$ with the right-hand side of equation (1) in (3)

$$[S(\mathbf{q}) + A(\mathbf{q})]\,[\mathbf{f}(\mathbf{q}) + N(\mathbf{q})\xi(t)] = -\nabla\phi(\mathbf{q}) + \hat{N}(\mathbf{q})\xi(t). \tag{5}$$

The *second* assumption is the separated equality of the deterministic and stochastic dynamics in equation (5)

$$[S(\mathbf{q}) + A(\mathbf{q})]\,\mathbf{f}(\mathbf{q}) = -\nabla\phi(\mathbf{q}), \tag{6}$$

$$[S(\mathbf{q}) + A(\mathbf{q})]\,N(\mathbf{q}) = \hat{N}(\mathbf{q}). \tag{7}$$

Intuitively, this assumption on separation is plausible for two different reasons: *first*, the zero mean noise function is nowhere differentiable but the deterministic forces are usually smooth (C^{∞}) functions, and hence two very different mathematical objects; *second*, the stochastic force and the deterministic forces describe different timescales of a physical system with different physical origins. By replacing equation (6) with an equivalent form (8) and plugging equations (7) and (2) into (4), we obtain the potential condition (8) and the generalized Einstein relation equation (9)

$$\nabla \times \{[S(\mathbf{q}) + A(\mathbf{q})]\,\mathbf{f}(\mathbf{q})\} = 0, \tag{8}$$

$$[S(\mathbf{q}) + A(\mathbf{q})]D(\mathbf{q})[S(\mathbf{q}) - A(\mathbf{q})] = S(\mathbf{q}). \tag{9}$$

In principle, the potential function $\phi(\mathbf{q})$ can be derived analytically by solving the $n(n-1)/2$ partial differential equations (under proper boundary conditions) of equation (8),

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together with the $n(n+1)/2$ equations given by equation (9) (n^2 unknowns in $[S(\mathbf{q})+A(\mathbf{q})]$ and n^2 equations). It can also be calculated numerically through a gradient expansion [6]. Detailed results near fixed points can be found in [9]. Explicit constructions of potential functions for limit cycles are contained in [17, 20].

In the one-dimensional case, $A = 0$, let $\epsilon = k_{\mathrm{B}}T$, if the friction γ is a constant, then $S = \gamma/k_{\mathrm{B}}T$, equation (9) reduces to $SD = \gamma D/k_{\mathrm{B}}T = 1$, namely, the product of the friction and diffusion coefficients is a constant, discovered by Einstein [31] one hundred years ago. Equation (9) is a generalized form of the Einstein relation in two ways: the diffusion matrix can be nonlinearly dependent of the state variable (a verification experiment has been reported [32]) and the detailed balance condition can be broken ($A(\mathbf{q}) \neq 0$, see also section 2.2.2).

From the generalized Einstein relation equation (9), we know that the symmetric part of $[S(\mathbf{q}) + A(\mathbf{q})]^{-1}$, $D(\mathbf{q}) = 1/2[(S(\mathbf{q}) + A(\mathbf{q}))^{-1} + ((S(\mathbf{q}) + A(\mathbf{q}))^{-1})^{\tau}]$, is the diffusion matrix defined in equation (2). Hence we have $[S(\mathbf{q}) + A(\mathbf{q})][D(\mathbf{q}) + Q(\mathbf{q})] = I$ (I is the identity matrix, singularity of $D(\mathbf{q})$, $S(\mathbf{q})$ or $A(\mathbf{q})$ can usually be tolerated), where $Q(\mathbf{q})$ is antisymmetric. Rewriting equation (6) as

$$\mathbf{f}(\mathbf{q}) = -\left[D(\mathbf{q}) + Q(\mathbf{q})\right] \nabla\phi(\mathbf{q}), \tag{10}$$

and by multiplying $\nabla\phi(\mathbf{q})$ on both sides of equation (10), we reach the Hamilton–Jacobi equation

$$\mathbf{f}(\mathbf{q}) \cdot \nabla\phi(\mathbf{q}) + \nabla\phi(\mathbf{q}) \cdot D(\mathbf{q}) \cdot \nabla\phi(\mathbf{q}) = 0. \tag{11}$$

Finally, using the knowledge from statistical physics, we can consider that the potential function leads to a Boltzmann–Gibbs distribution

$$\rho_s(\mathbf{q}) = \frac{1}{Z(\epsilon)} \exp\left(-\frac{\phi(\mathbf{q})}{\epsilon}\right), \tag{12}$$

as the steady state distribution (if it exists) for the stochastic process described by equation (3): ϵ as the 'temperature' and $\phi(\mathbf{q})$ as the 'Hamiltonian'. Experimental verification is available for some cases, e.g. [18].

Hence, the two assumptions to implement the equivalence between equations (1) and (3) lead to a potential function for the general Langevin equation and to a corresponding Boltzmann–Gibbs distribution for the final steady state independent of both matrices $A(\mathbf{q})$ and $S(\mathbf{q})$. While such a distribution function seems special, it should be pointed out that it is one of the most successful equations in physics, even broader than that of the stationary Schrödinger equation. The framework can be applied for systems with an arbitrary noise strength: equations (8) and (9) do not contain ϵ. In particular, deterministic systems can be regarded as the weak noise limit ($\epsilon \to 0$) of stochastic systems. The framework can also be extended directly to include parameter dependent potential and corresponding dynamical components [13, 20], e.g. time t and temperature ϵ dependent $\phi(\mathbf{q}, t, \epsilon)$. We note that equations (6) and (9) have a close connection to Lyapunov's direct method in engineering [17]. This evidence makes the assumptions more plausible and appealing.

This construction further leads to a stochastic integration (A-type) different from conventional ones such as Itô or Stratonovich. One may enquire about the mathematical consistency in this new approach. We point out that the consistency of A-type integration may be seen from two aspects. *First*, equation (1) or (3) by themselves are not complete descriptions of a stochastic process. A proper stochastic interpretation is needed, hence

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A-type is possible in principle. *Second*, we will show in the next subsection that there is an important situation in which one starts without the need to differentiate various known stochastic integrations, and reaches the consequence that an A-type interpretation is the natural choice for the SDE equations (3) and (1).

2.2. Demonstration of consistency

In this section, we summarize the main steps to demonstrate that A-type integration is mathematically consistent. The rationale is as follows. The starting point is the important stochastic differential equation in physics, Newton equation in $2n$ dimensions with noise and friction. Its corresponding $2n$-dimensional Fokker–Planck equation (FPE) is uniquely determined, known as the generalized Klein–Kramers equation. The valuable feature here is that all approaches to stochastic integration discussed in the present paper lead to the same $2n$-dimensional FPE. When taking the zero mass limit, the $2n$-dimensional Newton equation reduces to an n-dimensional equation in exactly the same form as equation (3), while the corresponding n-dimensional FPE derived from the generalized Klein–Kramers equation has the ability to permit the Boltzmann–Gibbs distribution as its stationary solution. After this zero mass limit, the connection between the resulting n-dimensional FPE and the stochastic differential equation is the A-type integration.

2.2.1. The generalized Klein–Kramers equation. We begin with a general situation via doubling the degrees of freedom, the $2n$-dimensional equation with noise, proposed in [6],

$$\begin{aligned} \dot{\mathbf{q}} &= \frac{\mathbf{p}}{m}, \\ \dot{\mathbf{p}} &= -[S(\mathbf{q}) + A(\mathbf{q})]\frac{\mathbf{p}}{m} - \nabla_{\mathbf{q}}\phi(\mathbf{q}) + \hat{N}(\mathbf{q})\xi(t), \end{aligned} \tag{13}$$

where $S(\mathbf{q})$, $A(\mathbf{q})$, $\phi(\mathbf{q})$, $\hat{N}(\mathbf{q})$ and $\xi(t)$ are identical to those in equation (3), and the subscript of $\nabla_{\mathbf{q}}$ means that it operates on $\mathbf{q}$ only, the same as in equation (3). We note that equation (13) has two properties: *first*, by taking the zero mass limit $m \to 0$, $\mathbf{p} \to 0$, we can recover equation (3) from (13); *second*, we wish to emphasize that starting with equation (13), we can find that different stochastic interpretations, Itô, Stratonovich, or A-type, will reach the same result, since $\nabla_{\mathbf{p}} \cdot [S(\mathbf{q}) + A(\mathbf{q})] = 0$.

The probability density function in the $(\mathbf{q}, \mathbf{p})$ phase space can be calculated through the path integral as

$$\rho(\mathbf{q}, \mathbf{p}, t) \equiv \langle \delta\left(\mathbf{q} - \bar{\mathbf{q}}\left(t, \{\xi(t)\}\right)\right) \delta\left(\mathbf{p} - \bar{\mathbf{p}}\left(t, \{\xi(t)\}\right)\right)\rangle, \tag{14}$$

where $\bar{\mathbf{q}}(t, \{\xi(t)\})$ and $\bar{\mathbf{p}}(t, \{\xi(t)\})$ represent the solution of the ordinary differential equation (ODE) reduced from equation (13) under a fixed sample path $\{\xi(t)\}$ of the sample space of $\xi(t)$ (a given noise configuration). By taking a partial derivative of time on both sides of equation (14), we obtain

$$\begin{aligned} \partial_t \rho &= \left\langle \nabla_{\bar{\mathbf{q}}} \delta\left(\mathbf{q} - \bar{\mathbf{q}}\right) \cdot \frac{\mathrm{d}\bar{\mathbf{q}}}{\mathrm{d}t} \delta\left(\mathbf{p} - \bar{\mathbf{p}}\right) + \delta\left(\mathbf{q} - \bar{\mathbf{q}}\right) \nabla_{\bar{\mathbf{p}}} \delta\left(\mathbf{p} - \bar{\mathbf{p}}\right) \cdot \frac{\mathrm{d}\bar{\mathbf{p}}}{\mathrm{d}t} \right\rangle \\ &= -\int \delta\left(\mathbf{q} - \bar{\mathbf{q}}\right) \delta\left(\mathbf{p} - \bar{\mathbf{p}}\right) \left\{ \nabla_{\bar{\mathbf{q}}} \cdot \left[\dot{\bar{\mathbf{q}}} P(\{\xi\})\right] + \nabla_{\bar{\mathbf{p}}} \cdot \left[\dot{\bar{\mathbf{p}}} P(\{\xi\})\right] \right\} \mathrm{d}\{\xi\} \end{aligned}$$

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$$= -\nabla_{\mathbf{q}} \cdot \frac{\mathbf{p}}{m}\rho - \nabla_{\mathbf{p}} \cdot \Big\{ -[S(\mathbf{q}) + A(\mathbf{q})] \cdot \frac{\mathbf{p}}{m}\rho - \nabla_{\mathbf{q}}\phi(\mathbf{q})\rho$$
$$+ \ \hat{N}(\mathbf{q}) \langle \xi(t) \delta(\mathbf{q} - \bar{\mathbf{q}})\, \delta(\mathbf{p} - \bar{\mathbf{p}}) \rangle \Big\}, \tag{15}$$

in which ρ, $\bar{\mathbf{q}}$ and $\bar{\mathbf{p}}$ have the same meanings as in equation (14), and $P(\{\xi\})$ is the probability density function for the given noise configuration $\{\xi(t)\}$. From step 1 to step 2 of equation (15), integration by parts is used. According to the Novikov identity [33], for a given functional $f[\xi(t), t]$ of noise $\xi(t)$,

$$\langle \xi(t) f[\xi(t), t] \rangle = \int \langle \xi(t) \xi^{\tau}(t') \rangle \left\langle \frac{\delta f[\xi(t), t]}{\delta \xi(t')} \right\rangle \mathrm{d}t'$$
$$= \left\langle \frac{\delta f[\xi(t), t]}{\delta \xi(t)} \right\rangle, \tag{16}$$

and using

$$\frac{\delta[\int_0^t \xi(t')\,\mathrm{d}t']}{\delta \xi(t)} = \frac{1}{2}, \tag{17}$$

noting that the solution of equation (13) can be expressed as

$$\bar{\mathbf{q}}(t) = \mathbf{q}(0) + \int_0^t \frac{\bar{\mathbf{p}}}{m}\,\mathrm{d}t', \tag{18}$$

$$\bar{\mathbf{p}}(t) = \mathbf{p}(0) + \int_0^t \left\{ -[S(\bar{\mathbf{q}}) + A(\bar{\mathbf{q}})] \frac{\bar{\mathbf{p}}}{m} - \nabla_{\bar{\mathbf{q}}}\phi(\bar{\mathbf{q}}) + \hat{N}(\bar{\mathbf{q}})\xi(t') \right\} \mathrm{d}t', \tag{19}$$

we obtain the relations

$$\frac{\delta \bar{\mathbf{q}}(t)}{\delta \xi(t)} = 0, \tag{20}$$

$$\frac{\delta \bar{\mathbf{p}}(t)}{\delta \xi(t)} = \frac{1}{2}\hat{N}^{\tau}(\bar{\mathbf{q}}). \tag{21}$$

The last left term in equation (15) can be handled as

$$\hat{N}(\mathbf{q}) \langle \xi(t) \delta(\mathbf{q} - \bar{\mathbf{q}})\, \delta(\mathbf{p} - \bar{\mathbf{p}}) \rangle = -2\epsilon S(\mathbf{q}) \cdot \tfrac{1}{2}\nabla_{\mathbf{p}}\rho. \tag{22}$$

We finally reach the generalized version of the Klein–Kramers equation [2]

$$\partial_t \rho = \nabla_{\mathbf{p}} \cdot \left\{ [A(\mathbf{q}) + S(\mathbf{q})] \cdot \frac{\mathbf{p}}{m} + \nabla_{\mathbf{q}}\phi(\mathbf{q}) + \epsilon S(\mathbf{q}) \cdot \nabla_{\mathbf{p}} \right\} \rho - \frac{\mathbf{p}}{m} \cdot \nabla_{\mathbf{q}}\rho. \tag{23}$$

Note that equation (23) has a solution (if the partition function $Z(\epsilon)$ is finite)

$$\rho_s(\mathbf{q}, \mathbf{p}) = \frac{1}{Z(\epsilon)} \exp\left(-\frac{p^2/2m + \phi(\mathbf{q})}{\epsilon} \right). \tag{24}$$

Equation (24) is not explicitly time dependent, $\partial_t \rho_s = 0$, it is a steady state distribution. The state variables $\mathbf{q}$ and $\mathbf{p}$ are separated, which simplifies the process of taking zero mass limit to be discussed below.

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2.2.2. Zero mass limit. We have mentioned that after taking zero mass limit $m \to 0$, equation (13) reduces to equation (3). Therefore, by acting the same limit process on equation (23), the corresponding FPE to equation (3) can be obtained [10],

$$\partial_t \rho(\mathbf{q}, t) = \nabla \cdot [D(\mathbf{q}) + Q(\mathbf{q})] \cdot [\epsilon \nabla + \nabla \phi(\mathbf{q})] \rho(\mathbf{q}, t), \tag{25}$$

where $D(\mathbf{q})$ is the diffusion matrix, $Q(\mathbf{q})$ is defined in equation (10), $\nabla \equiv \nabla_{\mathbf{q}}$, and the derivative ∇ in $\nabla\phi(\mathbf{q})$ does not operate on $\rho(\mathbf{q}, t)$. This FPE has a drift velocity $-[D(\mathbf{q}) + Q(\mathbf{q})]\nabla\phi(\mathbf{q}) = \mathbf{f}(\mathbf{q})$ and a generalized symmetric form $\nabla \cdot [D(\mathbf{q}) + Q(\mathbf{q})] \cdot \epsilon \nabla \rho(\mathbf{q}, t)$. The commonly defined probability current density $\mathbf{j}(\mathbf{q}, t) = (j_1(\mathbf{q}, t), \ldots, j_n(\mathbf{q}, t))^\tau$ is

$$j_i(\mathbf{q}, t) = (f_i + \Delta f_i)(\mathbf{q}) \rho(\mathbf{q}, t) - \partial_j \left[\epsilon D_{ij}(\mathbf{q}) \rho(\mathbf{q}, t)\right], \tag{26}$$

where $\mathbf{f}(\mathbf{q}) = (f_1(\mathbf{q}), \ldots, f_n(\mathbf{q}))^\tau$, $\Delta f_i(\mathbf{q}) = \epsilon \partial_j [D_{ij}(\mathbf{q}) + Q_{ij}(\mathbf{q})]$ (see also section 3.2), with $i = 1, \ldots, n$ and $j = 1, \ldots, n$, $D_{ij}(\mathbf{q})$ the ith-row and jth-column element of the diffusion matrix $D(\mathbf{q})$, and $Q_{ij}(\mathbf{q})$ the element of $Q(\mathbf{q})$ in equation (25). For steady state, equation (12), $\nabla \cdot \mathbf{j}_s(\mathbf{q}) = 0$. One can calculate that when $Q = 0$ then $\mathbf{j}_s = 0$; if $Q(\mathbf{q}) \neq 0$ then generally $\mathbf{j}_s(\mathbf{q}) \neq 0$, since $\partial_j [Q_{ij}(\mathbf{q}) \rho_s(\mathbf{q})] \neq 0$. Therefore the framework encompasses the cases without detailed balance. The term 'detailed balance' used here is defined for abstract phase space, that is, the net current between any two states in the phase space is zero [34], identical to that for the Markov process in mathematics.

There are various ways to take the zero mass limit (eliminate the fast degrees $\mathbf{p}$). A derivation adopting the standard projection operator method [1] is given in [10], that is, to project the $(\mathbf{q}, \mathbf{p})$ space to the $\mathbf{q}$ space. We note that another commonly used approach of degree reduction, adiabatic elimination [1, 4, 35], is based on the postulation that the velocity is a fast variable, which is consistent with the zero mass limit. Three other derivations for one-dimensional systems are discussed in [11]. This FPE (equation (25)) defines the A-type integration for an SDE of the form of equation (3). Since generally equation (1) is equivalent to equation (3), equation (25) defines a stochastic integration for general Langevin equations. The steady state distribution in the phase space (if it exists) is the Boltzmann–Gibbs distribution, equation (12). We should clarify that this is not to say that A-type is the only way to integrate equation (3), but it is a stochastic interpretation with physical significance.

3. Discussion

3.1. The physical meaning of equation (3)

We can consider a time evolution system described by an SDE as a particle motion inside the phase space. From a physical point of view, the motion of an object should be driven by some underlying forces. We consider this particle as a charged and *massless* one driven by the force $\mathbf{F}_{\text{total}} = m\ddot{\mathbf{q}} = 0$ $(m = 0)$. The driving force can be separated generally in physics into three parts, dissipative, conservative and random

$$\mathbf{F}_{\text{total}} = \mathbf{F}_{\text{dissipative}} + \mathbf{F}_{\text{conservative}} + \mathbf{F}_{\text{random}} = 0. \tag{27}$$

Equation (3) has exactly this structure. In the usual study of two- and three-dimensional cases, equation (3) corresponds to a known fundamental equation in physics. We can generally use a frictional force as the dissipative component: $\mathbf{F}_{\text{dissipative}} = -S(\mathbf{q})\dot{\mathbf{q}}$,

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where $S(\mathbf{q})$ is symmetric and positive semi-definite; and a Lorentz force together with an energy induced force (for example, the electrostatic force) as the conservative component, $\mathbf{F}_{\text{conservative}} = e\dot{\mathbf{q}} \times \mathbf{B}(\mathbf{q}) + [-\nabla\phi(\mathbf{q})]$; the random component is described by a Gaussian white noise $\mathbf{F}_{\text{random}} = \hat{N}(\mathbf{q})\xi(t)$ with zero mean that has a common origin with the frictional force, as formulated by the fluctuation-dissipation theorem [36]–[38], $\hat{N}(\mathbf{q})\hat{N}^{\tau}(\mathbf{q}) = 2\epsilon S(\mathbf{q})$, hence

$$-S(\mathbf{q})\dot{\mathbf{q}} + e\dot{\mathbf{q}} \times \mathbf{B}(\mathbf{q}) - \nabla\phi(\mathbf{q}) + \hat{N}(\mathbf{q})\xi(t) = 0. \tag{28}$$

The friction matrix $S(\mathbf{q})$ is positive semi-definite (guaranteed by the fluctuation-dissipation theorem), keeping the resistant property of the dissipative force (the allowed values are confined in the negative half space). It can be a non-diagonal matrix, describing an anisotropic frictional force. The potential function $\phi(\mathbf{q})$ plays a similar role to the Hamiltonian in dissipative systems, leading to a Boltzmann–Gibbs distribution on the final steady state (if it exists) of the stochastic process. For higher dimension, we generalize $\mathbf{B}(\mathbf{q}) \times \dot{\mathbf{q}}$ as $A(\mathbf{q})\dot{\mathbf{q}}$, where $A(\mathbf{q})$ is an antisymmetric matrix. There is a direct and simple physical realization based on this intuitive explanation of the SDE (3); for instance, practical experiments to verify the generalized Einstein relation were designed in section 5.3 of [13]. A recent experiment [18] has been implemented under a similar physical setting.

3.2. Difference and relation of the A-type integration with traditional ones

We have mentioned that the A-type integration reduces to an α-type one with $\alpha = 1$ for a one-dimensional system, hence it is different from Itô or Stratonovich's integration. A more detailed demonstration of this point is provided in [11]. For general cases, when the dimension is higher than one, things become more complicated: A-type integration is not even α-type, which means that at different time intervals the choices of α are not the same, or the parameter α is position dependent, $\alpha(\mathbf{q})$. A relation between A-type integration and Itô integration is formulated in [16] by considering the correspondence of their FPEs; that is, the SDE

$$\dot{\mathbf{q}} = (\mathbf{f} + \Delta\mathbf{f})(\mathbf{q}) + N(\mathbf{q})\xi(t), \tag{29}$$

where $\Delta\mathbf{f}(\mathbf{q}) = (\Delta f_1(\mathbf{q}), \ldots, \Delta f_n(\mathbf{q}))^{\tau}$, using Itô integration describes the same process as that of the SDE

$$\dot{\mathbf{q}} = \mathbf{f}(\mathbf{q}) + N(\mathbf{q})\xi(t) \tag{30}$$

using A-type integration. Here $\Delta f_i(\mathbf{q}) = \epsilon\partial_j[D_{ij}(\mathbf{q}) + Q_{ij}(\mathbf{q})]$. We note that there is an obvious distinction between $\Delta\mathbf{f}(\mathbf{q})$ here and the additional (to Itô's) drift term for α-type (α chosen as a constant) integrations $\Delta f_i^{(\alpha)}(\mathbf{q}) = \alpha[\partial_k N_{ij}(\mathbf{q})]N_{kj}(\mathbf{q})$.

An illustrative example has been provided in [16] to show a significant difference in the final steady state distributions between Itô and A-type integrations, the dynamics $\dot{\mathbf{q}} = \mathbf{f}(\mathbf{q}) + N(\mathbf{q})\xi(t)$ is

$$\begin{aligned} \dot{x} &= 2x - x\left(x^2 + y^2\right) + \sqrt{x^2 + y^2}\xi_x(t), \\ \dot{y} &= 2y - y\left(x^2 + y^2\right) + \sqrt{x^2 + y^2}\xi_y(t), \end{aligned} \tag{31}$$

2(x^2+y^2)

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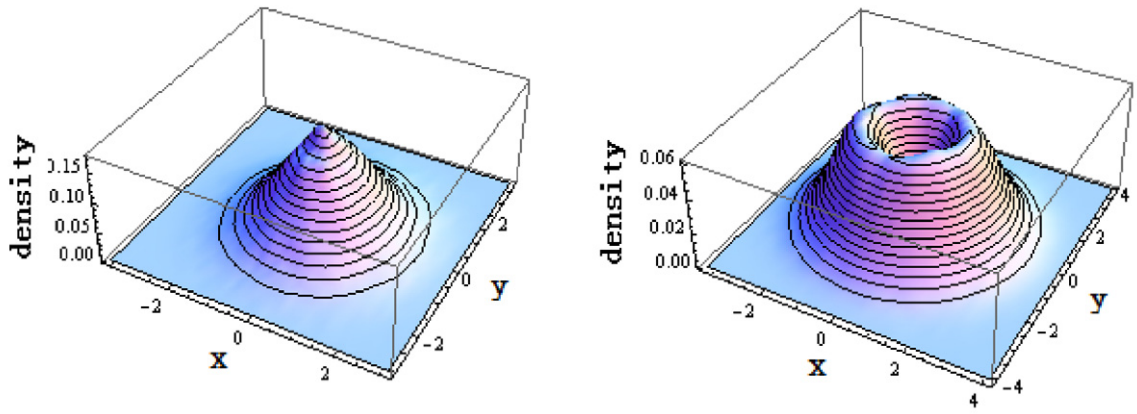

(a) (b)

Figure 1. Sampling results: the figure shows the distributions in the phase space for the long-term sampling of equation (31) using Itô and A-type integrations; the basal plane denotes the two-dimensional phase space and the vertical axis indicates the emerging probability density of the system at a specific state. (a) Itô integration. This is consistent with the theoretical result $\rho_{sI}(x, y) \propto \exp[-\psi/\epsilon]$ (ψ is given in equation (34), with $(0, 0)$ being the most probable state). (b) A-type integration. This is coherent with the deterministic dynamics obtained when $\epsilon = 0$; for example, it is most probable on the circle $x^2 + y^2 = 2$ (which represents stable fixed points when $\epsilon = 0$), and has zero probability at $(0, 0)$ (which is an unstable fixed point when $\epsilon = 0$).

=1

with $\mathbf{q} = (x, y)^\tau$, $\epsilon = \frac{1}{2}$, the diffusion matrix $D(x, y) = (x^2 + y^2)I_2$, $\xi(t) = (\xi_x, \xi_y)^\tau$ has zero mean, and $\langle \xi(t)\xi^\tau(t')\rangle = \delta(t - t')I_2$. The final steady state distribution of this system with A-type integration can be calculated based on the framework as $\rho_{sA}(x, y) = (1/Z_A(\epsilon)) \exp[-\phi/\epsilon]$ with

$$\phi(\mathbf{q}) = -\ln\left(x^2 + y^2\right) + \frac{x^2 + y^2}{2}. \tag{32}$$

The distribution of Itô integration for this system, $\mathbf{f} = \mathbf{f}' + \Delta\mathbf{f}$, is identical to the A-type distribution for the dynamics $\mathbf{f}'$ (in order to apply the result provided in equations (29) and (30), we decompose the original system $\mathbf{f}$ (equations (31)) into the form $\mathbf{f}' + \Delta\mathbf{f}$)

$$\begin{aligned} \dot{x} &= -x\left(x^2 + y^2\right) + \sqrt{x^2 + y^2}\xi_x(t), \\ \dot{y} &= -y\left(x^2 + y^2\right) + \sqrt{x^2 + y^2}\xi_y(t), \end{aligned} \tag{33}$$

2(x^2+y^2)

whose expression can be similarly calculated as $\rho_{sI}(x, y) = (1/Z_I(\epsilon)) \exp[-\psi/\epsilon]$ with

$$\psi(\mathbf{q}) = \tfrac{1}{2}\left(x^2 + y^2\right). \tag{34}$$

The two distributions ρ_{sA} and ρ_{sI} have obvious differences; for instance, $\rho_{sA}(0, 0) = 0$ but the origin $(0, 0)$ is the most probable state for ρ_{sI}. These theoretical results have been verified by numerical experiments in [16] (shown in figure 1). Note that the potential $\phi(\mathbf{q})$ in equation (32) serves as a global Lyapunov function [17] for the deterministic dynamics (when $\epsilon = 0$) of the system equations (31). The Lie derivative [39] of $\phi(\mathbf{q})$ $(\nabla\phi(\mathbf{q}) \cdot \mathbf{f}(\mathbf{q}))$

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Table 1. Fokker–Planck equations and steady state distributions with $\epsilon = 1$.

α	Fokker–Planck equation	Steady state distribution
0	$\frac{\partial}{\partial t}\rho(q,t) = \left[\frac{\partial}{\partial q}\frac{\partial}{\partial q}D(q) + \frac{\partial}{\partial q}D(q)\phi(q)\right]\rho(q,t)$	$\frac{1}{Z_I}\left\{\frac{1}{D(q)}\exp\left[-\phi(q)\right]\right\}$
$\frac{1}{2}$	$\frac{\partial}{\partial t}\rho(q,t) = \left[\frac{\partial}{\partial q}D^{1/2}(q)\frac{\partial}{\partial q}D^{1/2}(q) + \frac{\partial}{\partial q}D(q)\phi(q)\right]\rho(q,t)$	$\frac{1}{Z_S}\left\{\frac{1}{D^{\frac{1}{2}}(q)}\exp\left[-\phi(q)\right]\right\}$
1	$\frac{\partial}{\partial t}\rho(q,t) = \left[\frac{\partial}{\partial q}D(q)\frac{\partial}{\partial q} + \frac{\partial}{\partial q}D(q)\phi(q)\right]\rho(q,t)$	$\frac{1}{Z_A}\exp\left[-\phi(q)\right]$

stays non-positive. Therefore, there is an exact correspondence between the deterministic dynamics and the steady state distribution derived using A-type integration for SDEs; for example, the stable fixed points are locally most probable states, in accordance with one's intuition. This direct correspondence cannot be kept by applying Itô or Stratonovich integration: after using Itô integration, the unstable point $(0,0)$ of equations (31) ($\epsilon = 0$) becomes stable in $\psi(\mathbf{q})$; moreover, stable points on $x^2 + y^2 = 2$ in equations (31) ($\epsilon = 0$) disappear in equation (34). The unique advantage of using A-type integration compared to Itô or Stratonovich integration is shown here. It enables a straightforward calculation of the transition probability from one fixed point to another after taking into account the noise influence for ODE models which is essential in many applications [5, 7, 8, 12, 14]. For Itô or Stratonovich integrations, this is not direct and can even be impossible, since one cannot recognize the original stable fixed points from the long time sampling distribution, like what is shown in this example.

3.3. One-dimensional example

A comprehensive discussion on one-dimensional systems has been given previously [11]. The corresponding FPEs and the steady state distributions for three different types of stochastic integration (contained in [11]) are listed in table 1. As has been shown in [40], there exist real processes choosing Stratonovich integration. A recent experiment [18] on a one-dimensional physical process suggested that A-type integration of the corresponding SDE is consistent with the experimental data. We show in the following that the zero mass limit is well established based on the physical setting of the experiment.

For the colloidal particle studied in [18], $\rho = 1510$ kg m^{-3}, $R = 655 \times 10^{-9}$ m, the volume $V = 4/3\pi R^3 = 4/3 \times \pi \times (655 \times 10^{-9})^3$ m^3 $= 1.18 \times 10^{-18}$ m^3 and the mass of the particle is $m = \rho V = 1510 \times 1.18 \times 10^{-18}$ kg $= 1.78 \times 10^{-15}$ kg. The symbol dt denotes the sampling time interval in [18]; within d$t \leq 10$ ms, the authors claim that 'the force acting on the particle can be treated as locally constant'. In different experiments, they choose dt around the magnitude of 1 ms.

We use the simplified formula for the friction coefficient from Mannella *et al*'s discussion of the same experiment [4], with $\eta = 8.5$ mPa s and $z_0 = 700$ nm,

$$\gamma(z) = 6\pi\eta R\frac{(z + z_0)}{z}. \tag{35}$$

For $z \to \infty$, we have $\gamma_\infty = 6\pi\eta R = 6\pi \times 8.5 \times 10^{-3} \times 655 \times 10^{-9}$ N s m^{-1} $= 1.1 \times 10^{-7}$ N s m^{-1}, then the time needed for the particle to return to equilibrium after being acted on by an external force $F(z)$ is $t(z) = [F(z)/\gamma(z)]/[F(z)/m] = m/\gamma(z)$, $t_\infty = m/\gamma_\infty =$

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$1.78 \times 10^{-15}/1.1 \times 10^{-7}$ s $= 1.6 \times 10^{-8}$ s $\ll 1 \times 10^{-3}$ s $= 1$ ms $\approx \mathrm{d}t$. In figure 2 of [18], for instance, at $z = 200$ nm, $\gamma(z) = 1.1 \times 10^{-7}$ N s m$^{-1} \times (200+700)/200 = 5.0 \times 10^{-7}$ N s m^{-1}. Since $\gamma(z)$ is always larger than γ_∞, then $t(z) < t_\infty \ll \mathrm{d}t$. We conclude that during the sampling time interval the particle has been in equilibrium, hence the mass can be considered as zero in the experiment, realizing the zero mass limit.

3.4. Previous attempts

Some related previous attempts have been discussed in our former works [6, 9, 13]. In this subsection we provide a brief summary. No effort is made to give a complete list, but we hope to have picked some of the major ones.

To the best of our knowledge, the one-dimensional case of the present framework, $\alpha = 1$ type integration, has been mathematically discussed by Wong and Zakai in the 1960s [41] (see also [9, 13]). Their work provided a method for $\alpha \in [0, 1]$.

From a physics perspective Grabert *et al* [42] provided a method for nonlinear irreversible processes, which was discussed by Graham in a long review which we commented on in [6]. Their method has a restriction based on the singularity of the diffusion matrix $D(\mathbf{q})$ (see equations 2.14–16 in [42]) and handles the phase variables separately according to a reversibility defined by this singularity. By contrast, our framework can be used directly for a given $D(\mathbf{q})$ in its general form without a separated treatment, a global potential is then obtained in the whole phase space.

Theoretical considerations for the situations with detailed balance have been proposed by Klimontovich [43] (see also [13]), while our approach applies to situations both with and without detailed balance. In the weak noise limit, previous works have reached the same Hamilton–Jacobi equation as our equation (11), the nondifferentiable potentials reported in [44, 45] are then included within our framework; moreover, our potential function is valid for an arbitrary noise strength. A major difference between our construction of the potential and those in the literature such as the Graham–Haken construction [46] is that no assumption on the stationary distribution function is needed in our approach in the limit $t \to \infty$. In particular, the potential in our framework can be time dependent (see also [6, 20]). Other results beyond Itô and Stratonovich have been proposed in [47]–[49].

4. Conclusion

Beginning with a $2n$-dimensional stochastic differential equation (SDE) system we derived a generalized Klein–Kramers equation. This is a Fokker–Planck equation (FPE) that can be obtained from the SDE system regardless the type of stochastic calculus used (Itô and Stratonovich integrations of this SDE are described by the same FPE). This provides a natural starting point to demonstrate the internal consistency of our approach. After taking the zero mass limit, the $2n$-dimensional SDE reduces to an n-dimensional structured form that is equivalent to the n-dimensional Langevin equation with multiplicative noise based on our assumption. The corresponding generalized Klein–Kramers equation turns out to be a new FPE. This limiting process defines a new type of stochastic integration (A-type) for Langevin equations different from traditional ones. During the demonstration of consistency, the Itô versus Stratonovich dilemma is not encountered. In addition, the new FPE is generally not reachable by the α-type integration

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in higher dimensions. The framework and the A-type stochastic integration are natural consequences under a physical view of the time evolution dynamics in the phase space. An attractive advantage of A-type integration is the correspondence between stochastic and deterministic dynamics. For example, fixed points are not changed; this is not the case in Itô or Stratonovich integration. As an illustration, experimental data demonstrate that a one-dimensional physical process realizes the zero mass limit and chooses A-type integration.

Acknowledgments

The authors would like to express their sincere gratitude for the inspiring discussions during the weekly group meetings on stochastic processes in biology and related fields, their appreciation for the valuable comments from an anonymous referee, and their apology for not being able to include a full list of previous works in the present brief paper on a specific approach. This work was supported in part by the National 973 Project No. 2010CB529200 (PA) and by the Natural Science Foundation of China No. NFSC91029738 (PA) and No. NFSC61073087 (RY).

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