On the Existence of Potential Landscape in the Evolution of Complex Systems

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Abstract

A recently developed treatment of stochastic processes leads to the construction of a potential landscape for the dynamical evolution of complex systems. Since the existence of a potential function in generic settings has been frequently questioned in literature, here we study several related theoretical issues that lie at core of the construction. We show that the novel treatment, via a transformation, is closely related to the symplectic structure that is central in many branches of theoretical physics. Using this insight, we demonstrate an invariant under the transformation. We further explicitly demonstrate, in one-dimensional case, the contradistinction among the new treatment to those of Ito and Stratonovich, as well as others. Our results strongly suggest that the method from statistical physics can be useful in studying stochastic, complex systems in general.

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I. INTRODUCTION

Stochastic differential equations (SDEs) were first introduced in studying Brownian motions originally discovered in biology [1, 2]. Other developments in complex systems, from Darwin's evolutionary theory [3], the dynamics of gene regulatory networks [4], the cycle kinetics in biochemical networks [5], to the landscape paradigm [6], all have suggested that SDE is a useful and effective mathematical description for a wide range of dynamical processes [2, 7]. A distinct difference between the SDEs from biology and those widely studied in classical physics, usually called Langevin equations, is the absence of the detailed balance condition in the former. Hence the existence of a potential landscape with both local and global meanings has been frequently called into doubt [8]. During the study of the robustness and stability of a genetic switch involved in phage lambda, a bacterium killing virus, one of us has discovered a mathematical structure embedded in the SDE. This structure allows a direct quantification of the global stability of systems with fluctuations. Such unique structure leads a transformation of a SDE to a mathematical form familiar to theoretical physicists. The transformed SDE has a potential function, a friction matrix, a transverse force, and a random noise, together with a relationship between the noise and the friction similar to the fluctuation-dissipation relation [9, 10]. These four dynamical components can be obtained constructively from a SDE.

The mathematical structure and related transformation have immediate applications. With the aid of this method, the outstanding problem of the stability in phage lambda genetic switch has been solved [4]. More specifically, the relative stability of two fixed points in a dynamical system, in the presence of noise, can be uniquely determined. The connections of this mathematical structure to physics, and detailed behaviors near a fixed point, stable or unstable, have been analyzed rather exhaustively [11]. However, it is also noticed that in more general situations, the new transformation may give a result different from the conventional ones from the traditional integration of a SDE, such as by the Ito integration or by the Stratonovich integration [9, 11]. The unique structure suggests yet another stochastic integration. The purpose of the present paper is to explore this suggestion and to put it into a statistical physics perspective. In this way the application of statistical physics to complex dynamics is explicitly suggested.

In the following, we first summarize in section II the transformation from the standard

SDE into the transformed stochastic differential equation. We point out an interesting invariant of the transformation in section III, suggesting that the transformation might have a deeper mathematical root. In section IV we explicitly demonstrate the transformation in a special one dimensional case, where analytical results have been known in literature. A comparison to the Ito and Stratonovich integrations is made. Implications to various realistic applications are discussed in section V, and we conclude in section VI. Some mathematical details are provided in the Appendix.

II. REVIEW OF THE TRANSFORMATION

Let us consider a system described by state vector, $q^{\tau} = (q_1, ..., q_n)$, in *n* dimensional phase space, \mathbb{R}^n . Here the superscript τ denotes the transpose. The dynamic equation describing the time evolution of the system is the usual Langevin like, standard SDE,

$$\dot{q} = f(q) + \zeta(q, t) , \qquad (1)$$

a shorthand writing for $dq_i/dt = f_i(q) + \zeta_i(q, t)$. Here $\zeta^{\tau}(q, t) = (\zeta_1(q, t), \dots, \zeta_n(q, t))$ denotes stochastic forces, assumed to be represented by Gaussian white noises, with zero mean, $\langle \zeta(q, t) \rangle = 0$, and variance

$$\langle \zeta(q,t)\zeta^{\tau}(q,t')\rangle = 2D(q)\delta(t-t') , \qquad (2)$$

where D is a positive semi-definite diffusion matrix. The angular brackets denote the average over noise distribution, and $\delta(t)$ is the Dirac delta function. The temperature in the present paper, whenever it can be defined, is always set to 1. This is equivalent to absorbing the temperature into the potential function to be discussed below.

It was noticed [9, 10, 11] that this equation may be transformed into the form

$$[S(q) + T(q)]\dot{q} = -\nabla\phi(q) + \xi(q,t) , \qquad (3)$$

where the matrix S is positive semi-definite and symmetric, the matrix T antisymmetric. In analogous to the overdamped Brownian system in physics, here $-S\dot{q}$ plays the role of a dissipative force with a non-negative energy dissipation rate $\dot{q}^{\tau}S\dot{q}/2$. The matrix T plays a role similar to that of a magnetic field. The potential function is $\phi(q)$. The new stochastic force $\xi^{\tau}(q,t) = (\xi_1(q,t), ..., \xi_n(q,t))$, which has the same origin as $\zeta(q,t)$, is chosen to satisfy

$$\langle \xi(q,t)\xi^{\tau}(q,t')\rangle = 2S(q)\delta(t-t') , \qquad (4)$$

with zero mean. The steady state distribution for Eq. (3), if exists, would be Boltzmann-Gibbs like

$$\rho(q, t = \infty) \propto \exp\{-\phi(q)\}.$$
(5)

The transformation from Eqs. (1) to (3) is rather remarkable in that the original SDE in Eq. (1), with no explicit potential function, is transformed into the dynamic equation in Eq. (3), governed by the potential ϕ , which can be obtained without actually solving the time-dependent equation. The usual assumption of zero probability current or detailed balance as the potential condition is not required in the passage from Eq. (1) to Eq. (3). As pointed out, the results obtained in this way rely on the partial differntial equation for the probability density, $\rho(q, t)$, that is different in general from those based on either Ito or Stratonovich stochastic integration. Thus several questions naturally arise: Can this difference be more clearly demonstrated? Are there further implications of this transformation? In the following we attempt to give an affirmative demonstration to those questions from two different angles: the invariant of the transformation and the treatments of SDE's.

III. INVARIANT OF THE TRANSFORMATION

Here we wish to point out an invariant for potential function during the transformation from Eq. (1) into (3) within the framework of Langevin equation, Eq.(6), and the Fokker-Planck equation (Klein-Kramers equation), Eq.(7), two of most important equations in the description of nonequilibrium processes in physics. This invariant suggests a generic nature of the present transformation deeply rooted in statistical physics.

Let us consider the following nonlinear stochastic dynamics familiar in physics, an example for noise acting only on half of state variables:

$$\begin{cases} \dot{q} = \frac{p}{m} \\ \dot{p} = -[S(q) + T(q)]\frac{p}{m} - \nabla_q \phi(q) + \zeta(q, t) \end{cases}$$

$$\tag{6}$$

Here q, p are *n*-dimensional vectors, m a parameter, S an $n \times n$ semi-positive definite symmetric matrix, T an $n \times n$ antisymmetric matrix, and ϕ a potential function. The subscript q in gradient indicates that it operates on q only. There is an additional relationship, due to Einstein, between the noise ζ and S: $\langle \zeta(q,t)\zeta^{\tau}(q,t')\rangle = 2S(q)\delta(t-t')$. This equation is the Kramers' dynamics in the standard Langevin form in physics [2].

The probability distribution function $\rho(q, t)$ corresponding to the dynamical equation satisfies the Fokker-Planck equation [12], or Klein-Kramers equation [2],

$$\left\{ \partial_t + \frac{p}{m} \cdot \partial_q + \overline{f}(q, p) \cdot \partial_p \\ -\partial_p^{\tau} S(q) \left[\frac{p}{m} + \partial_p \right] \right\} \rho(q, p, t) = 0.$$

$$(7)$$

Here $\overline{f}(q,p) = p^{\tau}T(q)/m - \phi_q(q)$ with $\phi_q(q) = \partial_q \phi(q)$.

A stationary state, while $\partial_t \rho = 0$, exists and can usually be reached after a long time of dynamical evolution. From the analogy to physics, the final distribution from this dynamics is given by the Maxwell-Boltzmann-Gibbs distribution:

$$\rho(q, p, t = \infty) \propto \exp\left\{-\left[\frac{p^2}{2m} + \phi(q)\right]\right\} .$$
(8)

There is a clear separation of variables q, p in the final distribution function. This suggests that the mass of the particle is not an essential quantify to determine the distribution in the q-space, a fact well known in classical statistical physics. Hence the validity of Eq. (5) is implied.

We note that Eq. (6) is in the form of Eq. (1). To be more suggestive, we rewrite Eq. (6) as

$$\dot{x} = \mathcal{F}(x) + \mathcal{Z}(x,t) \tag{9}$$

Here

$$x = \begin{pmatrix} q \\ p \end{pmatrix}$$

is a 2n-dimensional vector,

$$\mathcal{F}(x) = \begin{pmatrix} p/m \\ -[S(q) + T(q)]p/m - \nabla_q \phi(q) \end{pmatrix},$$

and

$$\mathcal{Z} = \begin{pmatrix} 0 \\ \zeta \end{pmatrix} \ .$$

The $2n \times 2n$ diffusion matrix \mathcal{D} is defined by

$$\langle \mathcal{Z}(x,t)\mathcal{Z}^{\tau}(x,t')\rangle = 2\mathcal{D}(x)\delta(t-t') , \qquad (10)$$

and is

$$\mathcal{D}(x,t) = \begin{pmatrix} 0 & 0\\ 0 & S(q) \end{pmatrix} . \tag{11}$$

The important question is whether we can obtain the corresponding form of Eq. (3):

$$[\mathcal{S}(x) + \mathcal{T}(x)]\dot{x} = -\nabla_x \Phi(x) + \Xi(x,t)$$
(12)

with the same prediction on the potential, that is, without any change in physics prediction. Here \mathcal{T} is a $2n \times 2n$ antisymmetric matrix and \mathcal{S} a $2n \times 2n$ positive semi-definite symmetric matrix. We also require

$$\langle \Xi(x,t)\Xi^{\tau}(x,t')\rangle = 2\mathcal{S}(x)\delta(t-t') , \qquad (13)$$

with zero mean of Ξ .

The answer is affirmative, demonstrating a very suggestive invariant of the transformation. We give the result here, which can be verified directly:

$$\mathcal{T}(x) = \begin{pmatrix} T(q) & I \\ -I & 0 \end{pmatrix} , \ \mathcal{S}(x) = \begin{pmatrix} S(q) & 0 \\ 0 & 0 \end{pmatrix} .$$
(14)

Here I is the $n \times n$ identity matrix. The corresponding expression for $\mathcal{D} + \mathcal{Q} = (\mathcal{S} + \mathcal{T})^{-1}$ is

$$Q(x) = \begin{pmatrix} 0 & -I \\ I & T(q) \end{pmatrix} , \qquad (15)$$

and \mathcal{D} is precisely given by Eq.(11). The potential is

$$\Phi(x) = \frac{p^2}{2m} + \phi(q) , \qquad (16)$$

also precisely the same as that before the transformation. Thus, once the form of Eqs. (3) and (6) are reached, further manipulation of equations according to the transformation does not change the physical prediction.

IV. TREATMENTS OF STOCHASTIC DIFFERENTIAL EQUATIONS

The kinetic momentum in Eq. (6) can be eliminated, resulting in the following equation:

$$m\ddot{q} = -[S(q) + T(q)]\dot{q} - \nabla_q \phi(q) + \xi(q, t) .$$
(17)

Apparently, one would be able to take a zero mass limit by setting the right hand side of Eq. (17) zero. Carrying out this procedure, we have, copying Eq. (3),

$$[S(q) + T(q)]\dot{q} = -\nabla_q \phi(q) + \xi(q, t) .$$
(18)

This can be converted into a more suggestive form, the standard form of SDE, copying Eq. (1):

$$\dot{q} = f(q) + \zeta(q, t) . \tag{19}$$

Here $f(q) = -[S(q) + T(q)]^{-1} \nabla_q \phi(q)$ and $\zeta(q, t) = [S(q) + T(q)]^{-1} \xi(q, t)$.

Now, in connection of the singular behavior of the zero mass limit, we are facing a choice on the proper way to carry out the integration of Eq. (19). Different stochastic integration method would give different final distribution, hence different physical prediction. Here we illustrate this situation by considering explicitly the one dimensional case, n = 1. Higher dimensional case will be considered elsewhere [29]. In one dimensional case, n = 1 and T = 0, and Eq. (3) or (19) becomes

$$\dot{q} = -D(q)\nabla\phi(q) + \zeta(q,t) , \qquad (20)$$

and S(q)D(q) = 1. We explore its three different integrations below.

I. Present process. If we follow a limiting process to reproduce the final steady state distribution, the dynamical equation in this limit would be

$$\partial_t \rho(q,t) = [\partial_q D(q)\partial_q + \partial_q D(q)\phi_q(q)]\rho(q,t) .$$
(21)

This is in the form of the celebrated Smoluchowski equation [13]. Three different derivations from Eq. (7) to Eq. (21) are provided in the Appendix. Thus, the present stochastic integration process overlaps with that of the Smoluchowski process of strong damping limit. The steady state distribution would be, if exists,

$$\rho(q, t = \infty) \propto \exp\{-\phi(q)\}, \qquad (22)$$

the same as in Eq. (5).

II. Ito process. The Ito stochastic integration [14] is a strict implementation of Markov process and a martingale: There is no memory effect of previous dynamics and there is no information from future. The usual differentiation and integration rules would not be directly applicable here. Fortunately, this case has been studied in great details. The corresponding Fokker-Planck equation is, from Eq. (20) [15]:

$$\partial_t \rho_I(q,t) = [\partial_q \partial_q D(q,t) + \partial_q D(q,t)\phi_q(q)]\rho_I(q,t) .$$
(23)

The subscript I indicates that Eq. (23) is in accordance with Ito process. The steady state distribution would be, if exists, The steady state distribution would be, if exists,

$$\rho_I(q, t = \infty) \propto \frac{1}{D(q)} \exp\{-\phi(q)\} .$$
(24)

III. Stratonovich process. In the Stratonovich stochastic integration, the usual differentiation and integration rules apply [16]. This implies that the stochastic process such specified is a Markov process but not a martingale. Again, the stochastic integration has been carried out, and the corresponding Fokker-Planck equation is, from Eq. (20) [17]:

$$\partial_t \rho_S(q,t) = [\partial_q D^{\frac{1}{2}}(q,t) \partial_q D^{\frac{1}{2}}(q,t) + \partial_q D(q,t) \phi_q(q)] \rho_S(q,t) .$$
(25)

Similarly, the subscript S indicates that Eq. (25) is in accordance with Stratonovich process. The steady state distribution would be, if exists, the steady state distribution would be, if exists,

$$\rho_S(q, t = \infty) \propto \frac{1}{D^{\frac{1}{2}}(q)} \exp\{-\phi(q)\}.$$
(26)

The above one-dimensional examples clearly show that the present treatment of SDE implied in the transformation may be regarded as another stochastic integration process. It can indeed produce results different from those of Ito or Stratonovich process. One way to understand this difference is to view the zero mass limit as a singular limit in which specific procedure must be identified in order to get a well-defined result. As explicitly demonstrated above, there are relative shifts of density peaks from one process to another. In addition, the positions of peaks of the distribution function may not coincide with those of zeros of the potential ϕ or the fixed points of f. We have observed such shifts during numerical and analytical study even when the diffusion matrix D is constant [18], that is, even when there is no difference among those of Ito and Stratonovitch, and more general considerations [19]. Similar shifts have also been observed before [20, 21]. They are associated with the absence of detailed balance: In the presence of detailed balance condition and with a constant diffusion matrix, all those stochastic treatments would lead to the same potential function.

V. DISCUSSIONS

With various limiting procedures to integrate the SDE of the form of Eq. (1), (19) or (20), which one would be right? The answer is, not surprisingly, the procedure has to be determined by the real problem at hand and any of them can be correct in a practical situation [2, 7, 12, 22]. We illustrate this point by examples.

It should emphasized that it has been shown mathematically that in general, non-white noise can be constructed and its limiting process can lead to different stochastic integration with different Wong-Zakai correction [19]. We also note, in the case of 1d, that the Eq. (22) corresponds to the choice of evaluating the function at the end of a time interval. Higher dimensional case would be different [29]. The Ito process, Eq.(23), is then a choice of initial point, without peering into future. The Stratonovich process, Eq.(25), is a choice of middle point.

It is evident that from the physics point of view the first process appears to be a natural choice: the presence of small mass limit encountered frequently. It results in the known Smoluchowski equation [2, 7, 12]. Numerous experiments in physics exist to support this approach. We wish to point out that the form of Eq. (6) allows a generalization into more complicated situations, such as the colored noise, as done in the dissipative dynamics [23, 24]. This is also the form used in a recent development of a mesoscopic, open-system nonequilibrium thermodynamics [25].

From an engineering point of view, everything would be thought as a limit of continuous process, hence Stratonovich process would be a natural choice. Indeed, analog experiments have been done to check this situation. The results are in remarkable agreement with the Stratonovich stochastic integration [26].

From a population geneticist's point of view, Ito process would appear more natural to model the population dynamics. Indeed this view has been carried out in detail [27, 28]. We are, however, not aware of any precise comparison between experimental/expirical data and the theoretical calculation which can single out the Ito process as the appropriate description in this case.

It is worthwhile to point out here that, in connection with the invariant discussed in section III, in the corresponding Fokker-Planck equation for Eq. (6), the Eq. (7), there is no need to differentiate all those stochastic processes discussed in section IV, because of the

special algebraic structure expressed in Eq. (11) and (14). This adds a further preference to view the present process as a "natural" one.

VI. CONCLUSION

In this paper we have given an explicit demonstration of the difference between the present integration of the stochastic differential equation and those according to classical methods in one dimension. While we believe all those integration methods are in themselves consistent, we do point point that the present process has a certain advantage, as demonstration by the invariant of the transformation and by the zero mass limit. Thus, the existence of potential landscape in complex systems is put on a firmer theoretical ground.

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Appendix: Three Derivations of Eq. (21)

The particular form of the partial differential equation in Eq.(21) has not been widely discussed in literature. Since it plays an important role in our study of the potential land-scape, we give three derivations which are not related to the usual treatments of stochastic differential equations [19]. An extension of Eq.(21) into higher dimensions is discussed in Ref.[10].

First derivation

Here we give some justifications, both physical and mathematical, to the derivation of the Eq. (21) in one dimension. The derivations for the equations (23) and (25) are well documented in the literature. Interested readers should consult textbooks such as that by van Kampen [2], Gardiner [7], or Risken [12].

We note that there is an alternative expression for Eq. (6)

$$\begin{cases} \dot{q} = v \\ m\dot{v} = -[S(q,t) + T(q,t)]v - \nabla_q \phi(q) + \zeta(q,t) \end{cases}$$
(27)

Eqs. (6) and (27) are for the inner and outer solutions to the problem with fast and slow

time scales respectively. In one dimensional case, n = 1 and T = 0, we may rewrite equation (7) as

$$\partial_t \rho(q, p, t) = \left(-\frac{p}{m} \partial_q + \phi_q(q) \partial_p + \partial_p S(q) \left[\frac{p}{m} + \partial_p \right] \right) \rho(q, p, t) .$$
(28)

The right hand side of Eq. (28) can be regrouped according to the following manner:

$$\begin{aligned} \partial_t \rho(q, p, t) \\ &= \left(\partial_p \left[S(q)\partial_p + S(q)\frac{p}{m}\right] + \partial_p \phi_q(q) - \frac{p}{m}\partial_q\right)\rho(q, p, t) \\ &= \left(\left[\partial_p - \partial_q \frac{1}{S(q)}\right] \left[S(q)\partial_p + S(q)\frac{p}{m}\right] \\ &+ \partial_q \frac{1}{S(q)} \left[S(q)\partial_p + S(q)\frac{p}{m}\right] + \partial_p \phi_q(q) - \frac{p}{m}\partial_q\right)\rho(q, p, t) \\ &= \left(\left[\partial_p - \partial_q \frac{1}{S(q)}\right] \left[S(q)\partial_p + S(q)\frac{p}{m}\right] \\ &+ \partial_p \left[\partial_q + \phi_q(q)\right]\right)\rho(q, p, t) \\ &= \left(\left[\partial_p - \partial_q \frac{1}{S(q)}\right] \left[S(q)\partial_p + S(q)\frac{p}{m} + \phi_q(q) + \partial_q\right] \\ &+ \partial_q \frac{1}{S(q)} \left[\partial_q + \phi_q(q)\right]\right)\rho(q, p, t) . \end{aligned}$$
(29)

There are two lines of attack for this problem in the literature. One was taken by Kramers himself and Chandrasekhar [1], the other is based on the projection operator approach [7]. The essential assumption in the latter approach is that the momentum p stationarity is achieved instantaneously when the mass m is small. It takes the time of order m/S(q)for it to reach equilibrium. Because we are interested in the dynamics on the time scale $\Delta t \gg m/S(q)$, we may regard the dynamics of the kinetic momentum p is in an instantaneous equilibrium with the dynamics of the coordinate q. We may then assume the trial solution for the distribution function in the following form:

$$\rho(q, p, t) = \rho(q, t)\rho_K(p, t|q) , \qquad (30)$$

with conditional probability of p given q:

$$\rho_K(p,t|q) = \sqrt{\frac{1}{2\pi m}} \exp\left\{-\frac{1}{2m} \left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right)^2\right\}$$
(31)

Here $\Delta \phi(q) = -\ln \rho(q, t) - \phi(q)$ and $\Delta \phi_q(q) = \partial_q \Delta \phi(q)$. The distribution of kinetic momentum is Gaussian, in the familiar form of kinetic energy. At a given moment the average kinetic momentum is not zero, corresponding to the drifting velocity $\Delta \phi_q(q)/S(q)$. The drifting velocity is zero at the eventual equilibrium state, as would expected. We expect that the error raised from this choice will be in the higher order of m/S(q) comparing to what would be kept. We will show below that it is indeed the case.

With the trial solution the contribution of the first term of the right hand side of Eq. (29) is:

$$K = \left[\partial_{p} - \partial_{q} \frac{1}{S(q)} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} + \phi_{q}(q) + \partial_{q} \right] \rho(q,t)\rho_{K}(p,t|q) \\ = \rho(q,t) \left[\partial_{p} - (-\Delta\phi_{q}(q) - \phi_{q}(q) + \partial_{q})\frac{1}{S(q)} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} + \phi_{q}(q) \\ + (-\Delta\phi_{q}(q) - \phi_{q}(q) + \partial_{q}) \right] \rho_{K}(p,t|q) \\ = \rho(q,t) \left[\partial_{p} - (-\Delta\phi_{q}(q) - \phi_{q}(q) + \partial_{q})\frac{1}{S(q)} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \rho_{K}(p,t|q) \\ = \rho(q,t) \left[\partial_{p} - (-\Delta\phi_{q}(q) - \phi_{q}(q) + \partial_{q})\frac{1}{S(q)} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} - \Delta\phi_{q}(q) + \partial_{q} \right] \times \left[S(q)\partial_{p} + S(q)\frac{p}{m} + \Delta\phi_{q} \right] + \left[S(q)\partial_{p} + S(q)\frac{p}{m} + \Delta\phi_{q} \right] + \left[S(q)\partial_{q} + S(q)\frac{p}{m} - \Delta\phi_{q} \right] + \left[S(q)\partial_{q} + S(q)\frac{p}{m} + \Delta\phi_{q} \right] + \left[S(q$$

Moving ρ_K from the right to left, and grouping all terms, we have

$$K = \rho(q,t) \times \sqrt{\frac{1}{2\pi m}} \exp\left\{-\frac{1}{2m} \left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right)^2\right\} \times \left[-\frac{1}{m} \left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right) - \left(-\Delta\phi_q(q) - \phi_q(q) - \frac{1}{m} \left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right) \partial_q \left(\frac{m\Delta\phi_q(q)}{S(q)} + \partial_q\right)\right) \frac{1}{S(q)}\right] \times \left[-S(q)\frac{1}{m} \left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right) + S(q)\frac{p}{m} - \Delta\phi_q(q) - \frac{1}{m} \left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right) \partial_q \left(\frac{m\Delta\phi_q(q)}{S(q)}\right)\right]$$
(33)
$$= \rho(q,t) \times \sqrt{\frac{1}{2\pi m}} \exp\left\{-\frac{1}{2m} \left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right)^2\right\} \times \left[-\frac{1}{m} \left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right) \left(1 + \left(\partial_q \left(\frac{m\Delta\phi_q(q)}{S(q)}\right)\right) - \partial_q\right) \frac{1}{S(q)}\right) - \left(-\Delta\phi_q(q) - \phi_q(q)\right)\right] \times \left[-\frac{1}{m} \left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right) \partial_q \left(\frac{m\Delta\phi_q(q)}{S(q)}\right)\right] .$$

Performing integration over p, all linear terms are zero, we have

$$\int_{-\infty}^{\infty} dp \ K = \rho(q, t) \left(1 + \left(\partial_q \left(\frac{m \Delta \phi_q(q)}{S(q)} \right) \right) - \partial_q \right) \frac{1}{S(q)} \right) \\
= \frac{m}{S(q)} \rho(q, t) \left[S(q) \left(1 + \left(\partial_q \left(\frac{m \Delta \phi_q(q)}{S(q)} \right) \right) - \partial_q \right) \frac{1}{S(q)} \right) \partial_q \left(\frac{\Delta \phi_q(q)}{S(q)} \right) \right] \\
= O\left(\frac{m}{S(q)} \right) \rho(q, t) \\
\rightarrow 0,$$
(34)

when $\frac{m}{S(q)} \to 0$. Note that $\rho(q,t) = \int_{-\infty}^{\infty} dp \ \rho(q,p,t)$, integrating Eq. (29) over p, we have

$$\partial_t \rho(q,t) = \left(\partial_q \frac{1}{S(q)} \left[\partial_q + \phi_q(q)\right]\right) \rho(q,t) .$$
(35)

This is Eq. (21). The correction is in higher order of m/S. This completes our first derivation of Eq.(21).

Second derivation

We can also follow the original approach of Kramers for the derivation of Eq. (35), our second derivation of Eq.(21). One subtle issue in this approach is realizing that to obtain $\hat{\rho}(q,t)$ from $\rho(q,p,t)$, one needs to integrate out p along the curve q + p/S = constantin which (p/m) is the velocity and m/S is the relaxation time for the velocity. For any v on the order 1, of course, this correction is on the order of m/S. For non-constant S(q), the derivation presented below is in close parallel to that of Kramers, but with extra mathematical complications.

We first observe several mathematical relations.

(A.i) From distribution $\rho(x, y)$, the distribution for z = x + ay is $\int \rho(z - ay, y) dy$.

(A.ii) We have an identity

$$\left(\partial_v - \partial_q \left(\frac{m}{S(q)} \right) \right) \Psi(q, p) \Big|_{mv = z - \int S(q) dq}$$

$$= \partial_q \overline{\Psi} \left(q, \frac{z}{m} - \frac{1}{m} \int S(q) dq \right)$$

$$(36)$$

in which $\overline{\Psi}(q, v) = -m\Psi(q, v)/S(x)$. (A.iii) Let $v = \frac{1}{m} \left(z - \int S(q) dq \right)$ and its inverse function be q = g(z - mv). Then we have, for any G

$$\frac{1}{m} \int_{-\infty}^{\infty} dq \ G\left(q, \frac{1}{m} \left(z - \int S(q) dq\right)\right) \\
= \int_{-\infty}^{+\infty} dv \frac{G(g(z - mv), v)}{S(g(z - mv))} \\
\rightarrow \int_{-\infty}^{+\infty} \left[dv \frac{G(q, v)}{S(q)} \right]_{q = g(z)}$$
(37)

when $m \to 0$.

Starting with the SDE in Eq. (27), we have equation similar to (29):

$$\frac{\partial_t \rho(q, v, t)}{= \left(\left[\partial_v - \partial_q \frac{m}{S(q)} \right] \left[\frac{S(q)}{m^2} \partial_v + \frac{vS(q) + \phi_q(q)}{m} + \frac{1}{m} \partial_q \right] \\
+ \partial_q \frac{1}{S(q)} \left[\partial_q + \phi_q(q) \right] \right) \rho(q, v, t) .$$
(38)

Define random variable $z = mv + \int S(q)dq$ and we have its distribution according to the relation (A.i),

$$\rho(z,t) = \frac{1}{m} \int_{-\infty}^{\infty} \rho\left(q, \frac{z}{m} - \frac{1}{m} \int S(q) dq\right) dq.$$
(39)

Using the above relations (A.ii) and (A.iii),

$$\begin{aligned} \partial_t \rho(z,t) \\ &= \frac{1}{m} \int_{-\infty}^{+\infty} dq \times \\ & \left[\partial_q \left(\frac{1}{S(q)} \partial_q + \frac{\phi_q(q)}{S(q)} \right) \rho(q,v,t) \right]_{v=\frac{1}{m} \left(z - \int S(q) dq \right)} \\ &\to \int_{-\infty}^{+\infty} \frac{dv}{S(q)} \left[\partial_q \left(\frac{1}{S(q)} \partial_q + \frac{\phi_q(q)}{S(q)} \right) \rho(q,v,t) \right]_{q=g(z)} \\ &= \frac{1}{S(q)} \left[\partial_q \left(\frac{1}{S(q)} \partial_q + \frac{\phi_q(q)}{S(q)} \right) S(q) \rho(z,t) \right]_{q=g(z)}. \end{aligned}$$

$$(40)$$

Finally, we note that if we define random variable $\zeta = g(u)$, then the distribution for ζ : $\rho_{\zeta}(y) = S(y)\rho_z \left(\int S(y)dy\right)$. In the limit of $m \to 0$, $\zeta = g\left(mv + \int S(q)dq\right) \to q$, and the distribution for ζ satisfies the equation:

$$\partial_t \rho(q,t) = \partial_q \left(\frac{1}{S(q)} \partial_q + \frac{\phi_q(q)}{S(q)} \right) \rho(q,t).$$
(41)

Again, this is Eq. (21).

Third derivation

It may appear that the first derivation is too intuitive and the second one is too formal. One may wonder whether or not there is a more programmatic derivation. The answer is positive. Here we give such one where the higher order correction in the small mass limit would be systematically obtained. The trial distribution function is assumed in Eqs. (30), (31). We show it is indeed the right solution from the Klein-Kramers equation in Eq. (28).

First we write

$$\rho(q, p, t) = \exp\left(-\Delta\phi(q) - \phi(q) - \frac{p^2}{2m} + A(q, p, t) + mB(q, p, t)\right)$$
(42)

The higher order terms in m are included in B(q, p, t). Then Eq. (28) gives

$$-\Delta\phi_{t} - \phi_{t} + A_{t} + mB_{t}$$

$$= \frac{p}{m}(\Delta\phi_{q} - A_{q}) - pB_{q} + \phi_{q}A_{p} + m\phi_{q}B_{p} + S(q)$$

$$\left(-\frac{p}{m}A_{p} - pB_{p} + A_{p}^{2} + 2mA_{p}B_{p} + m^{2}B_{p}^{2}\right)$$
(43)

where the subscripts denote the derivatives with respect to t, q, p. Then the term of $\mathcal{O}(1/m)$ yields

$$\Delta \phi_q - A_q - S(q)A_p = 0.$$
(44)

Then we can find A for small p, noting p is order of m.

$$A(q,p) = \frac{\Delta \phi_q}{S(q)} p + \mathcal{O}(p^2)$$
(45)

This satisfies Eq. (44) in the above, where A_q gives $\mathcal{O}(p)$. This justifies the trial form of the distribution function used in our first derivation. The rigorous solution for A(q, p) can be found:

$$A(q,p) = \left[1 - \exp\left(-\frac{p}{S(q)}\partial_q\right)\right]\Delta\phi\tag{46}$$

We will take only the first order in p. Nevertheless, we point out that this procedure can be carried out to higher orders by matching the corresponding orders in Eq. (43).

The expression corresponding to Eq. (33) should read as follows:

$$K = \rho(q,t) \times \sqrt{\frac{1}{2\pi m}} \exp\left\{-\frac{1}{2m}\left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right)^2\right\}$$
$$\times \left[-\frac{1}{m}\left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right) + \partial_p - \left\{-\Delta\phi_q(q) - \phi_q(q) + \frac{1}{m}\left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right) \partial_q\left(\frac{m\Delta\phi_q(q)}{S(q)}\right) + \partial_q\right\}\frac{1}{S(q)}\right]$$
$$\times \left[-\frac{S(q)}{m}\left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right) + S(q)\frac{p}{m} - \Delta\phi_q(q) + \frac{1}{m}\left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right) \partial_q\left(\frac{m\Delta\phi_q(q)}{S(q)}\right)\right]$$
$$= \rho(q,t) \times \sqrt{\frac{1}{2\pi m}} \exp\left\{-\frac{1}{2m}\left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right)\partial_q\left(\frac{m\Delta\phi_q(q)}{S(q)}\right)^2\right\}$$
$$\times \left[\left\{-\frac{1}{m}\left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right)\left(1 + \frac{1}{S(q)}\partial_q\left(\frac{m\Delta\phi_q}{S(q)}\right)\right) + (\Delta\phi_q + \phi_q - \partial_q)\frac{1}{S(q)}\right\}$$
$$\times \left\{\frac{1}{m}\left(p - \frac{m\Delta\phi_q(q)}{S(q)}\right)\partial_q\left(\frac{m\Delta\phi_q}{S(q)}\right)\right\}$$
$$+ \partial_q\left(\frac{\Delta\phi_q}{S(q)}\right)\right]. \tag{47}$$

According to this, Eq. (34) leads to:

$$\int_{-\infty}^{\infty} dp K = \rho(q, t) \left[-\frac{1}{m} \left\{ 1 + \frac{1}{S(q)} \partial_q \left(\frac{m \Delta \phi_q}{S(q)} \right) \right\} \\ \partial_q \left(\frac{m \Delta \phi_q}{S(q)} \right) + \frac{m}{S(q)} \left\{ \partial_q \left(\frac{\Delta \phi_q}{S(q)} \right) \right\}^2 \\ + \partial_q \left(\frac{\Delta \phi_q}{S(q)} \right) \right] \\ = 0 .$$
(48)

It is exactly zero, not approximate zero as in Eq. (34) Again, Eq. (21) follows in the zero mass limit.

Above demonstration evidently indicates that the novel stochastic integration procedure discussed in the present paper has a strong connection to the overdamping dynamics, the Smoluchowski limit. They are the same in one dimension, but differ generally in higher dimensional cases which would be addressed elsewhere.

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 Based on an extession of one of the three demonstrations in above Appendix.
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