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Citation: J. Chem. Phys. **145**, 147104 (2016); doi: 10.1063/1.4964681
View online: http://dx.doi.org/10.1063/1.4964681
View Table of Contents: http://aip.scitation.org/toc/jcp/145/14
Published by the American Institute of Physics

THE JOURNAL OF CHEMICAL PHYSICS **145**, 147104 (2016)

Comment on "Construction of the landscape for multi-stable systems: Potential landscape, quasi-potential, A-type integral and beyond" [J. Chem. Phys. 144, 094109 (2016)]

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(Received 5 April 2016; accepted 12 July 2016; published online 14 October 2016)

[http://dx.doi.org/10.1063/1.4964681]

Recently Zhou and Li (ZL)[1] extensively discussed connections among three known ways of finding potential landscapes for generic nonequilibrium processes in biology, chemistry, engineering, and physics described by stochastic differential equations (SDEs). Some interesting questions were formulated, along with a few insightful results. They speculated that a set of differential equations proposed 10 years ago, referred to as "SDE decomposition" by ZL, would have generally no unique solution. In this comment, we show that such speculation is not supported by either mathematical or physical reasoning. A few more points raised by ZL are further clarified.

We first show mathematically ZL's "non-uniqueness proof" is invalidated by counterexamples. The existence and uniqueness of the "SDE decomposition" have been explicitly and rigorously demonstrated for a class of important stochastic processes: linear stochastic processes including those of Ornstein-Uhlenbeck. Note that these systems are covered by ZL's "non-uniqueness proof." If the drift term $\mathbf{f}(\mathbf{q}) = F\mathbf{q}$ and any two eigenvalues λ_i and λ_j of the matrix F satisfying $\lambda_i + \lambda_j \neq 0$, the existence and uniqueness of $[S + A]$ (S and A are independent of state variable provided as a boundary condition) in the whole state space are guaranteed by a theorem on Lyapunov equation.[2,3] The condition $\lambda_i + \lambda_j \neq 0$ is actually not essential as already demonstrated[4] and an explicit expression was obtained. Hence, the speculation on the general non-uniqueness by ZL is incorrect.

The uniqueness of the "SDE decomposition" may be suggested from physics side, too. The two fluctuation-dissipation relations[5] $\sigma(\mathbf{q})\sigma(\mathbf{q})^t = 2\varepsilon D(\mathbf{q})$ and $\tilde{\sigma}(\mathbf{q})\tilde{\sigma}(\mathbf{q})^t = 2\varepsilon S(\mathbf{q})$ define the diffusion matrix $D(\mathbf{q})$ and the friction matrix $S(\mathbf{q})$, respectively. The transverse matrix $A(\mathbf{q})$ can be related to an effective magnetic field. The physical meanings of $S(\mathbf{q})$ and $A(\mathbf{q})$ were apparently not used by ZL. They can be in principle measured independently. It is unlikely in a real physical process that two sets of results could be obtained.

The "SDE decomposition"[6,7] decomposes an SDE into three components: a potential function $\phi(\mathbf{q})$ (a scalar function), a friction matrix $S(\mathbf{q})$ (symmetric and semi-positive definite), and a conservative force represented by a transverse matrix $A(\mathbf{q})$ (antisymmetric). Matrices $S(\mathbf{q})$ and $A(\mathbf{q})$ are determined by the potential condition (Eq. (1a)) and the generalized Einstein relation (Eq. (1b)),

$$\nabla \times \{[S(\mathbf{q}) + A(\mathbf{q})]\,\mathbf{f}(\mathbf{q})\} = 0, \tag{1a}$$

$$[S(\mathbf{q}) + A(\mathbf{q})]D(\mathbf{q})[S(\mathbf{q}) - A(\mathbf{q})] = S(\mathbf{q}), \tag{1b}$$

where $\mathbf{f}(\mathbf{q})$ is the deterministic drift velocity and $D(\mathbf{q})$ the diffusion matrix given by the SDE. The $\nabla \times \mathbf{x} = \partial_i x_j - \partial_j x_i$ for arbitrary n-dimensional vector $\mathbf{x}$. In principle, the n^2 unknowns in $[S(\mathbf{q}) + A(\mathbf{q})]$ can be uniquely determined by solving the $n(n-1)/2$ partial differential equations (PDEs) in Eq. (1a) *under boundary conditions for matrices* $S(\mathbf{q})$ *and* $A(\mathbf{q})$ *set by the problem under study*, together with the $n(n+1)/2$ equations given by Eq. (1b) (n^2 unknowns and n^2 equations). Eqs. (1a) and (1b) are the same as Eqs. (28a) and (28b) in Ref. 1.

Equation (1) may be transformed into a more standard but equivalent form (when $[S + A]$ is invertible). Notice that Eq. (1b) implies a relation that $[S + A] = [D + Q]^{-1}$, where Q is an antisymmetric matrix. We therefore rewrite Eqs. (1a) and (1b) as

$$\nabla \times \left\{[D(\mathbf{q}) + Q(\mathbf{q})]^{-1}\mathbf{f}(\mathbf{q})\right\} = 0, \tag{2}$$

where the $n(n-1)/2$ PDEs determine the $n(n-1)/2$ unknowns in the antisymmetric matrix Q with necessary boundary conditions for Q. Based on the theory of PDE, the existence and uniqueness of solution are guaranteed at least locally[8] for this quasi-linear first order PDE.[9] It should be pointed out that such general reasoning for uniqueness was also used by ZL for the solution of the Hamilton-Jacobi Equation (HJE) for the potential function,[1,7]

$$\mathbf{f}(\mathbf{q}) \cdot \nabla\phi(\mathbf{q}) + \nabla\phi(\mathbf{q}) \cdot D(\mathbf{q}) \cdot \nabla\phi(\mathbf{q}) = 0. \tag{3}$$

In fact, ZL have already argued the general existence of the SDE decomposition. A proper boundary condition can then be found by iteratively narrow down a condition to eliminate multiple solutions. For real systems, such a boundary condition for uniqueness may be naturally obtained. With the existence and uniqueness of SDE decomposition settled generally, we turn to the toy model of a diffusion process on the circle $\mathcal{S}[0, 1]$ in ZL.[1] We noted that it indeed reveals an additional feature largely overlooked, apparently even not noticed by ZL: The steady state distribution is generally not determined by the potential function in the form of Boltzmann-Gibbs distribution. There is no question to have

Hamiltonian or potential function for dissipative dynamics in such a situation,[10] and the steady state distribution can even be exactly evaluated.[11] The mathematical reason of this mismatch is that Eq. (1a) is sensitive to the topological constraint in the state space.[12] In fact, the potential function can be formulated in different ways when the steady state distribution stays the same: For the toy model, our Eq. (1) naturally generates two solutions (without specifying boundary condition), (i) $\phi'(x) = 0$, which leads to $\phi^{AO}(x) = constant$ (with $S = 0$ by (1b), and $D = 1$, $A \equiv 0$); (ii) a washboard potential $\phi(x) = -x$ (with $S = 1$ by (1b), and $D = 1$, $A \equiv 0$) that is well-known to exist in real physical systems.[11] These two solutions from our Eq. (1) nicely correspond to the two solutions of the HJE discussed by ZL:[1] $(1 + \phi'(x))\phi'(x) = 0$. In order to establish uniqueness for their quasi-potential, ZL also explicitly used a *boundary condition*; however, they generally eliminated the solution corresponding to the washboard potential, leading to failure in modeling certain physical systems.[11] We note that a proper boundary condition should be determined by the actual problem under study. Contrast to what ZL stated non-equivalence in their Table IV, this is an exactly demonstrable example of their asserted mathematical equivalence between the SDE decomposition and the Freidlin-Wentzell (F-W) formulation.

Having showed that ZL's non-uniqueness speculation is incorrect, several points raised in their paper deserve further discussion, clarification, or correction.

(i) Potential function is more generally applicable than the steady state distribution. In cases the steady state distribution does not exist, a potential function may still be obtainable. We had considered such a case recently.[13] It is our observation that this important feature has not been generally appreciated so far in the literature. This feature, together with the above discussion on the toy model, may lead to the conclusion that there is a serious limitation on the scope of its application for constructing potential function from steady state distribution.

(ii) ZL noticed that the HJE plays a central role in the "SDE decomposition," similar to that in F-W formulation. We are pleased to point out that such observation had been noticed by us, too.[7]

(iii) ZL proved that the singularity on D does not affect the decomposition framework. We have also noticed and stressed this feature,[7] which is evident from the SDE decomposition but less obvious in other formulations. For example, a naïve implementation of F-W formulation involved $1/D$ (cf. Eq. (12) of ZL), which apparently requires the non-singularity of D.

(iv) ZL inappropriately referred the fluctuation-dissipation theorem[5] $\tilde{\sigma}(\mathbf{q})\tilde{\sigma}(\mathbf{q})^t = 2\varepsilon S(\mathbf{q})$ as the generalized Einstein relation (1b).

(v) ZL stated that for SDE decomposition, "there is no explicit stochastic integral interpretation of it in higher dimensions." It is an incorrect assertion. The zero mass limit justification[14] of SDE decomposition is in fact an explicit realization of stochastic integration in two steps: first, the usual stochastic integration, such as Ito type, and then the zero mass limit. Because the implicit doubling of dimension of state space, it is not the usual stochastic integration in a standard textbook, as we have already recognized as beyond Ito vs Stratonovich.[7] It is possible that a more conventional interpretation may be found.

(vi) ZL asked the important question of how to generalize what has been obtained for continuous processes to discrete jump processes and speculated that the "SDE decomposition" theory would be difficult to do that. We had in fact showed that the generalization is possible.[15] Such generalization is a direct extension of the "SDE decomposition."

(vii) The starting point of ZL's "non-uniqueness proof" is not the definition of the "SDE decomposition" by Eq. (1): their protocol ignored necessary boundary conditions for the dynamical matrices S, A, and Q. Two different types of physically realizable boundary conditions are discussed above. It appears as an open mathematical question that how many types of consistent boundary conditions may exist for Eq. (2) or (3).

To summarize, while ZL reported many interesting observations, their non-uniqueness speculation is not only un-rigorous, but it is also incorrect.

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