

Self-contained framework of stochastic mechanics for reconstructing the Onsager-Machlup theory

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The two different forms of stochastic Lagrangian in the literature which stem from a common deterministic model $L(\dot{\mathbf{x}}, \mathbf{x}, t) = \frac{1}{2}m\dot{\mathbf{x}}^2 + \mathbf{A}(\mathbf{x}, t) \cdot \dot{\mathbf{x}} - V(\mathbf{x}, t)$ are analyzed referring to the question Nelson raised in his recent book *Quantum Fluctuations*, and a resolution is presented. It is argued that there exists a self-contained framework of stochastic mechanics, different from Nelson's original proposal, which is prescribed by (i) $\mathbf{a} = \frac{1}{2}(DD + D_*D_*)\mathbf{x}$ for the stochastic acceleration, (ii) the same procedure as Nelson of connecting both sides of the stochastic differential equation for the process $\mathbf{x}(t)$ with the current and osmotic velocities but with entirely real-valued wave functions, and (iii) a special relation between V and \mathbf{A} which conforms the above L to the Onsager-Machlup Lagrangian.

The notion of stochastic mechanics was introduced by Nelson^{1,2} to discuss a rederivation of the Schrödinger equation for (nonrelativistic) quantum mechanics. He proposed a series of mathematically satisfactory steps to deduce this equation by combining the two well-established frames of classical physics, namely, Newtonian mechanics and the theory of diffusion processes, anticipating that by this combination the long historical endeavors to understand quantum mechanics in pure classical languages, apart from the physical postulate of introducing the Planck constant, could become one of the major theoretical disciplines in physics. Stochastic mechanics, according to Nelson, is not just the usual mathematical tool of describing diffusion processes, because it includes a prescription of how to reverse the time axis of the diffusions and how to associate the acceleration of the pertinent Brownian particle with a mechanical force acting on it. These may be summarized by the stochastic Newton's law

$$m\mathbf{a} = \mathbf{F} \tag{1}$$

(with an appropriate stochastic definition of the \mathbf{a}). We see from the literature, in fact, that Nelson's reconstruction of quantum mechanics has attracted interest and been extended steadily in the last decade under the name of "stochastic quantization."³

Up to the present, the terminology "stochastic mechanics" has been used almost exclusively in accordance with Nelson to imply a basic framework on which quantum mechanics is to be reconstructed. Here, I wish to point out the existence of another framework which is entirely self-contained to say, "it is nothing to do with quantum mechanics;" instead, to say, "a basic framework on which nonequilibrium thermodynamics could be formulated." By this terminology I mean that the dynamics is described in part by an explicit use on the probability concept for a system, and in part purely thermodynamically for the background to which the system is in contact; the same conception as "mesoscopic level of description," as is exemplified by van Kampen.⁴ A direct use of this framework is the construction of a satisfactory formulation of the Onsager-Machlup theory⁵ beyond linear (Gaussian) processes.

I have been motivated by Nelson's⁶ lectures as an extended version of his original work,^{1,2} in particular, from the

viewpoint of the variational principles pertaining to stochastic mechanics, where two recent important contributions to the subject have been cited and discussed, namely, *stochastic calculus of variation* by Yasue⁷ and *quantization of dynamical systems and stochastic control theory* by Guerra and Morato.⁸

Nelson⁹ noticed the two different choices of the stochastic Lagrangian for the variational principle adopted in the above two papers which are incompatible with each other, expressing his desire to understand the reason for this difference, and also noting that Yasue's choice naturally leads to the original definition^{1,2} of the stochastic acceleration \mathbf{a} in the Newtonian law (1), i.e.,

$$\mathbf{a} = \frac{1}{2}(D_*D + DD_*)\mathbf{x} \tag{2}$$

where D and D_* imply the well-known (again, what Nelson introduced) mean forward and backward derivation in time, respectively, applied to any quasimartingale process.

In reply to Nelson's question, I would like specifically to note that the other choice of the stochastic Lagrangian adopted by Guerra and Morato,⁸ when set in the variational principle that is compatible with Yasue's procedure,⁷ leads us to another definition of the stochastic acceleration, denoted by $\bar{\mathbf{a}}$ to be distinguished from (2); thus

$$\bar{\mathbf{a}} = \frac{1}{2}(DD + D_*D_*)\mathbf{x} \tag{3}$$

Note that the possibility of defining the stochastic acceleration in this form was mentioned by Nelson at the beginning of his work² in connection with the Einstein-Smoluchowski process for overdamped oscillators, and that later Davidson¹⁰ noted the nonuniqueness of \mathbf{a} by mixing the term (3) with the original definition (2) to derive the unique Schrödinger equation. It would be of interest to investigate the consequence of (3), when incorporated into Nelson's other prescriptions, to obtain another framework of "stochastic mechanics."

Specifically, let us consider a modified stochastic Newtonian equation,

$$\frac{1}{2}(DD + D_*D_*)\mathbf{x} = \frac{1}{m}\mathbf{F} = 2\nu \left[\mathbf{v} \times \text{curl} \mathbf{A} - \frac{\partial \mathbf{A}}{\partial t} - \nabla V \right] \tag{4}$$

where the inverse mass is replaced by twice the diffusion coefficient ν (a single scalar, > 0),¹¹ which is compared with

$$\frac{1}{2}(D_*D + DD_*)\mathbf{x} = \frac{1}{m} \left[\mathbf{v} \times \text{curl} \mathbf{A} - \frac{\partial \mathbf{A}}{\partial t} - \nabla V \right], \quad (5)$$

considered first by Nelson for deriving the Schrödinger equation. Thus, a combination of Eq. (4) with both-sided stochastic differential equations

$$d\mathbf{x} = \mathbf{b}(\mathbf{x}(t), t) dt + d\mathbf{w}(t) \quad (6a)$$

$$= \mathbf{b}_*(\mathbf{x}(t), t) dt + d\mathbf{w}_*(t) \quad (6b)$$

under the Gaussian white-noise assumptions for $\mathbf{w}(t)$ and $\mathbf{w}_*(t)$ with strength 2ν , together with Nelson's rest prescriptions about the current and osmotic velocities relat-

$$i\hbar \frac{\partial \psi}{\partial t} = \left[\frac{1}{2m} \left(\frac{\hbar}{i} \nabla - \mathbf{A}(\mathbf{x}, t) \right) \cdot \left(\frac{\hbar}{i} \nabla - \mathbf{A}(\mathbf{x}, t) \right) + V(\mathbf{x}, t) \right] \psi, \quad (8a)$$

$$-i\hbar \frac{\partial \psi^*}{\partial t} = \left[\frac{1}{2m} \left(\frac{\hbar}{-i} \nabla - \mathbf{A}(\mathbf{x}, t) \right) \cdot \left(\frac{\hbar}{-i} \nabla - \mathbf{A}(\mathbf{x}, t) \right) + V(\mathbf{x}, t) \right] \psi^*, \quad (8b)$$

and also on the possible physical significance to be assigned to such equations.

It is not difficult to obtain the desired pair of evolution equations if one examines and precisely follows Nelson's procedure to deduce Eqs. (8a) and (8b) from his original scheme of stochastic mechanics. The first step is to write the evolution equations for the osmotic and current velocities which must be integrable and replaceable by a set of two equations for the two scalar fields: The probability density ρ and the *action* S , which have been introduced in the latter part of Eqs. (7a) and (7b). Hence, one proceeds to the second step of examining this set. It is equivalent to Bohm's representation of quantum mechanics,¹² i.e., the equation of continuity and the Hamilton-Jacobi equation with the scalar potential being supplemented by an additional term called the "quantum-mechanical potential." In the latter step, it is crucial to recognize that only the necessary modification caused by the replacement of the stochastic acceleration \mathbf{a} in (2) by $\bar{\mathbf{a}}$ in (3) is a sign change of this extra potential (equivalent to the sign change of the osmotic part in the stochastic Lagrangian,⁶ or to considering this part as a part of the potential energy rather than the kinetic one⁸). This can be seen explicitly from

$$\frac{\partial \rho}{\partial t} + \text{div}(\mathbf{v}\rho) = 0 \quad (9a)$$

[the current velocity \mathbf{v} in (7a)], and

$$\frac{\partial S}{\partial t} + \nu(\nabla S - \mathbf{A})^2 + V + \nu\rho^{-1/2}\Delta\rho^{1/2} = 0, \quad (9b)$$

where the last term in (9b) should be replaced by the quantum-mechanical potential $(-\hbar^2/2m)\rho^{-1/2}\Delta\rho^{1/2}$ (besides $\nu = 1/2m$ in the kinetic part), if the above equation were for quantum mechanics discussed by Bohm.¹²

The sign change of the additional potential mentioned above caused by the ansatz (3) for the modified acceleration

ed to the two drifts \mathbf{b} and \mathbf{b}_* , i.e.,

$$\mathbf{v}(\mathbf{x}, t) = \frac{1}{2}[\mathbf{b}(\mathbf{x}, t) + \mathbf{b}_*(\mathbf{x}, t)] \equiv \nu(\nabla - \mathbf{A}), \quad (7a)$$

$$\mathbf{u}(\mathbf{x}, t) = \frac{1}{2}[-\mathbf{b}(\mathbf{x}, t) + \mathbf{b}_*(\mathbf{x}, t)] \equiv \nu\nabla\rho, \quad (7b)$$

is just the framework of stochastic mechanics which I propose to analyze.

Since the above formulation of "stochastic mechanics" does not involve any fundamental constant in physics other than the arbitrary positive constant of diffusion ν , the resulting framework must be entirely independent of quantum mechanics, i.e., of the Schrödinger equation which we know is derivable from a similar formulation, when Eq. (4) is replaced by (5) and the white-noise strength 2ν by \hbar/m , the Planck constant divided by $2\pi m$. Hence, our interest may be focused on the pair of Schrödinger-type equations of evolution prescribed by Eqs. (4), (6a), (6b), (7a), and (7b) together with a judicious choice of a "wave function," as compared with

should necessitate an alteration in defining the "wave function" to get a set of linear evolution equations: $\rho = \psi^*\psi$, $S = -\frac{1}{2} \ln \psi/\psi^*$. This amounts to deleting the imaginary unit i everywhere in the transformation between the Schrödinger and Bohm representations [the action S thereby is a dimensionless quantity consistent with (4)], discarding, at the same time, the assignment of the asterisk to denote complex conjugation. For the purpose of uniqueness, therefore, let us assume a restriction that all "wave functions" so introduced are real. The resulting evolution equations for $\psi = \sqrt{\rho}e^{-S}$ and for $\psi^* = \sqrt{\rho}e^S$ are found to be

$$\frac{\partial \psi}{\partial t} = \nu(\nabla + \mathbf{A}) \cdot (\nabla + \mathbf{A})\psi + V\psi, \quad (10a)$$

$$-\frac{\partial \psi^*}{\partial t} = \nu(-\nabla + \mathbf{A}) \cdot (-\nabla + \mathbf{A})\psi^* + V\psi^*. \quad (10b)$$

We note that the two linear operators acting on ψ and ψ^* on the right-hand sides of the above equations are not generally self-adjoint but can be adjoint to each other in the usual L_2 - (real) Hilbert space, provided the real vector and scalar potentials \mathbf{A} and V satisfy certain conditions (such as with a compact support). Thus, the asterisk on ψ to give ψ^* may still retain the meaning of the Hilbert-space adjoint.

Consequently, the derived Schrödinger-type equations are nothing but the Fokker-Planck equation for (10a) and the backward equation of Kolmogorov for (10b), iff

$$V = -\nu\mathbf{a}^2 + \nu \text{div} \mathbf{A}. \quad (11)$$

By inserting this into Eqs. (10a) and (10b), in fact, it is easy to see that these equations become

$$\frac{\partial \psi}{\partial t} = \nabla \cdot (2\nu\mathbf{A}\psi) + \nu\Delta\psi, \quad (12)$$

$$-\frac{\partial \psi^*}{\partial t} = -2\nu\mathbf{A} \cdot \nabla\psi^* + \nu\Delta\psi^*,$$

i.e., the Fokker-Planck equation with the drift vector $-2\nu\mathbf{A}$ and its dual equation. It may be further remarked that the condition (11) of fixing the scalar potential in terms of the vector potential is equivalent to requiring either that ψ have the meaning of a probability density so that it obeys an equation of continuity (in the first equation in (12), $\partial\psi/\partial t + \text{div}[-2\nu\mathbf{A} - \nu\nabla \ln\psi]\psi = 0$), or that ψ^* satisfy Eq. (10b) so it is an identity by the special choice $\psi^* = 1$ [in the second equation in (12), there is no term other than derivatives of ψ^*]. This means that, for relation (11) to hold, the derived framework of the present stochastic mechanics contains two objects to which a probability density can be assigned: They are ρ and ψ , both being subject to an equation of continuity, i.e.,

$$\frac{\partial\rho}{\partial t} + \text{div}(\mathbf{v}\rho) = 0, \quad \mathbf{v} = -\nu\nabla \ln \frac{\psi}{\psi^*} - 2\nu\mathbf{A} \quad (13a)$$

$$\frac{\partial\psi}{\partial t} + \text{div}(\mathbf{v}_0\psi) = 0, \quad \mathbf{v}_0 = -\nu\nabla \ln\psi - 2\nu\mathbf{A} \quad (13b)$$

These two equations of continuity are identical, if and only

if $\psi^* = 1 \times \text{const.}$ It is noteworthy that according to this specialization the Hamilton-Jacobi equation (9b) also becomes identical to this equation of continuity (or, Fokker-Planck) for ψ .

The above remarks about the ‘‘coincidence’’ of two independent evolution equations (13a) and (13b), or (9a) and (9b) by specializing to $\psi^* = 1$, characteristic of any dissipative dynamics described by Fokker-Planck equations (more generally, of Markovian dynamics), should be important if one wishes to get general principles of such dynamics. Essentially, one wishes to formulate an intention expressed in the Onsager-Machlup theory, i.e., to achieve a stochastic understanding of the principle of least dissipation.⁵ Space prohibits going into details. Readers are referred to my previous publications.¹³ Here, I must restrict the discussion to the essential contrast between the two frameworks of stochastic mechanics: *quantum* and *dissipative dynamical*. Most of the formal points in the preceding discussion are listed in Table I, where a change of notations is made so that ψ is replaced by ρ (a single-gate probability density) and ψ^* by f

TABLE I. A comparison between the two prototype frameworks of stochastic mechanics.

	Quantum-mechanical framework	Dissipative-dynamical framework
Deterministic Lagrangian	$L(\dot{\mathbf{x}}, \mathbf{x}, t) = \frac{1}{2}m\dot{\mathbf{x}}^2 + \mathbf{A}(\mathbf{x}, t) \cdot \dot{\mathbf{x}} - V(\mathbf{x}, t)$	
Stochastic Lagrangian	$L_{st}(D\mathbf{x}D_*\mathbf{x}, \mathbf{x}, t) = \frac{m}{2} \frac{(D\mathbf{x})^2 + (D_*\mathbf{x})^2}{2} + \mathbf{A} \cdot \frac{1}{2}(D\mathbf{x} + D_*\mathbf{x}) - V$	$L_{st}(D\mathbf{x}D_*\mathbf{x}, \mathbf{x}, t) = \frac{1}{2}mD_*\mathbf{x} \cdot D\mathbf{x} + \mathbf{A} \cdot \frac{1}{2}(D\mathbf{x} + D_*\mathbf{x}) - V$ $m = (2\nu)^{-1}$
Stochastic Newtonian	$\frac{1}{2}(D_*D + DD_*)\mathbf{x} = \frac{1}{m}\mathbf{F}$	$\frac{1}{2}(DD + D_*D_*)\mathbf{x} = 2\nu\mathbf{F}$
White-noise strength	$E\mathbf{w}(t) \cdot \mathbf{w}(0) = E\mathbf{w}_*(t) \cdot \mathbf{w}_*(0) = \frac{\hbar}{m}\delta(t)$	$E\mathbf{w}(t) \cdot \mathbf{w}(0) = E\mathbf{w}_*(t) \cdot \mathbf{w}_*(0) = 2\nu\delta(t)$
Equation of continuity	$\frac{\partial\rho}{\partial t} + \text{div}(\mathbf{v}\rho) = 0, \quad \mathbf{v} = \frac{1}{m}(\nabla S - \mathbf{A})$	
Hamilton-Jacobi equation	$\frac{\partial S}{\partial t} + \frac{1}{2m}(\nabla S - \mathbf{A})^2 + V - \frac{\hbar^2}{2m}\rho^{-1/2}\Delta\rho^{1/2} = 0$	$\frac{\partial S}{\partial t} + \nu(\nabla S - \mathbf{A})^2 + V + \nu\rho^{-1/2}\Delta\rho^{1/2} = 0$
Scalar potential V	Independent of \mathbf{A}	$V = -\nu\mathbf{A}^2 + \nu \text{div}\mathbf{A}$
Schrödinger \rightleftharpoons Bohm transformation	$\psi = \sqrt{\rho}e^{(i/\hbar)S}, \quad \rho = \psi^*\psi,$ $\psi^* = \sqrt{\rho}e^{-(i/\hbar)S}, \quad S = \frac{\hbar}{2i} \ln \frac{\psi}{\psi^*}$	$\rho = \sqrt{\rho\rho_0}e^{-S}, \quad \rho = f\rho,$ $f = (\rho/\rho_0)^{1/2}e^S, \quad S = -\frac{1}{2} \ln \frac{\rho}{f\rho_0}$
Expectation of the Hamiltonian	$EH = \int [\frac{1}{2}m(\mathbf{v}^2 + \mathbf{u}^2) + V]\rho d\mathbf{x}$ (System energy)	$EH = \int \left\{ \frac{1}{4\nu}(\mathbf{v}^2 - \mathbf{u}^2) + V \right\} \rho d\mathbf{x}$ $\Phi(\text{flux}) - \Psi(\text{force})^a$

^aSee Ref. 5. This assumes time reversal. A general expression is in Ref. 13.

(an arbitrary dynamical quantity of the system). Note that with relation (11) the starting "classical" Lagrangian $L(\dot{\mathbf{x}}, \mathbf{x}, t) = \frac{1}{2}m\dot{\mathbf{x}}^2 + \mathbf{A} \cdot \dot{\mathbf{x}} - V$ becomes what has been called the Onsager-Machlup Lagrangian;¹⁴ $L = (1/4\nu)(\dot{\mathbf{x}} - \boldsymbol{\alpha})^2 + \frac{1}{2}\text{div}\boldsymbol{\alpha}$, if $m^{-1} = 2\nu$ and the drift vector $-2\nu\mathbf{A}$ is denoted by $\boldsymbol{\alpha}$.

Perhaps one significant point of the present discussion in reply to Nelson's question may be an adequate interpretation of the "action S ": Can an entropy concept for such nonequilibrium dynamics be assigned to this quantity, and, if so, how? At present, I can only say that the familiar H theorem can be formulated satisfactorily in the variational context by considering the mean forward derivative of $2S$, where the specialization $\psi^* = 1$ is necessary to realize the situation of steady approach of the system to an equilibrium state [see the argument after Eq. (14)]. For the formulation, one can exploit an analogy to a gauge transformation in the counterpart quantum mechanics. The quantum action S is indefinite to the addition of the gauge function for any gauge transformation, whereas the quantum probability density ρ is invariant under this transformation. For dissipative dynamics, the situation is the same: If the dynamics has an invariant measure, the log of its (probability) density may provide a satisfactory "gauge function," in terms of which the H theorem may be formulated for both time directions, realizing the concept of "mirror image" introduced by Onsager and Machlup.⁵

A crucial difference in understanding the role of probability density ρ between the two frameworks, in spite of the same equation of continuity, should be recognized. It is the well-known quantum probability density in the quantum-mechanical framework. What is it in the dissipative-dynamical framework? The answer is again well known in

the theory of Markov processes; a joint probability density (two-gate density according to Onsager and Machlup⁵), if space-time indices are explicitly given to ψ and ψ^* so that

$$\rho(\mathbf{x}, t) = \text{const} \times p(\mathbf{x}_2 t_2, \mathbf{x} t) p(\mathbf{x} t, \mathbf{x}_1 t_1), \quad t_1 < t_2. \quad (14)$$

Here, the equivalence of the equation of continuity for this ρ and the well-known Chapman-Kolmogorov composition formula should be observed, from which the normalization constant for $\int \rho d\mathbf{x} = 1$ is seen to be given by $\text{const} = p(\mathbf{x}_2 t_2, \mathbf{x}_1 t_1)^{-1}$. If this constant is absorbed into $\psi^*(\mathbf{x}, t) = p(\mathbf{x}_2 t_2, \mathbf{x} t)$, saying "specializing to $\psi^* = 1$ " should be fully understood. It is the expression of a steady approach of the system to equilibrium to be achieved, as a mathematical technique, by $t_2 \rightarrow \infty$.

The two assignments of physical meaning to the probability density ρ are very different for the two prototype stochastic mechanics, as we have just seen. This was my starting consideration when I attempted, some time ago,¹⁵ to explore the counter framework to Nelson's stochastic mechanics for quantum systems, and must be the crucial point of clarification if one anticipates a unified framework of both, such as by making the pertinent variables complex; the action S and the density ρ . Several open problems listed by Nelson⁶ (for example, a formulation of dissipative quantum mechanics) are expected in the scope of this unification.

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