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Stochastic Quantization and Detailed Balance in Fokker–Planck Dynamics

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The path integral and operator formulations of the Fokker–Planck equation are considered as stochastic quantizations of underlying Euler–Lagrange equations. The operator formalism is derived from the path integral formalism. It is proved that the Euler–Lagrange equations are invariant under time reversal if detailed balance holds and it is shown that the irreversible behavior is introduced through the stochastic quantization. To obtain these results for the nonconstant diffusion Fokker–Planck equation, a transformation is introduced to reduce it to a constant diffusion Fokker–Planck equation. Critical comments are made on the stochastic formulation of quantum mechanics.

KEY WORDS: Fokker–Planck equation; operator formalism; path integral; irreversibility; Lagrangian.

1. INTRODUCTION

Two different methods of dealing with the Fokker–Planck equation (FPE) are receiving increasing attention. The first is the path integral method pioneered by Onsager and Machlup[(1)] as a kinetic generalization of the Boltzmann–Einstein principle relating entropy to probability.[(2)] The probability distribution function for fluctuation paths is expressed in terms of a dissipation function which is in turn defined by means of the phenomenological kinetic equations.[(3–14)]

The second method for dealing with the FPE has its origin in the operator formulation[(15–16)] of the MSR formalism.[(17)] Operator equations of motion[(18–21)] are introduced for the set of gross variables describing the

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system under consideration. As a result the classical gross variables no longer commute at different times. This approach can be viewed as a kind of Heisenberg picture for stochastic dynamics in which the time dependence of the probability distribution function is transferred to the gross variables. In this picture, commutativity between gross variables at different times is precluded by the stochastic nature of the process.[21]

As an illustration of the practical importance of these methods we may cite the possibility of developing a consistent perturbation scheme[14,20–22] using the powerful techniques originally developed for quantum field theory.[23] A remarkable feature of the Onsager–Machlup path integral formulation is the fact that the probability distribution over paths can be expressed in terms of an action integral of a Lagrangian[3–14,24–27] for which the Euler–Lagrange equations are precisely the equations of motion of the Heisenberg picture. This result, first noted by Enz,[28] is rigorously true as long as these equations are interpreted as c-number equations. The extension of this result to the operator equations of motion needed to describe stochastic dynamics is not straightforward, however, as ordering ambiguities have been found to occur.[5,14,22,24,28]

The purpose of this paper is twofold. First, we wish to show how the ordering ambiguities may be dealt with by means of a consistent "stochastic quantization" procedure starting from a postulated path integral expression for the transition probability of a continuous Markov process or "diffusion process." By "stochastic quantization" we mean here the passage from c-number Euler–Lagrange equations to the operator equations describing stochastic dynamics. This should not be confused with Nelson's approach to quantum mechanics.[29–33] Emphasis is placed, not on the different possible definitions of the path integral,[14,24] but rather on the differences with the analogous quantum mechanical procedure and, in particular, on the non-equivalence between the forward and backward FPE, a feature which does not appear in quantum mechanics but which does here due to the asymmetry between initial and final states. Our approach to the stochastic quantization problem is developed in Section 2, where we derive the operator equations of the Heisenberg picture for stochastic dynamics from the path integral formulation.

Our second purpose is to analyze the origin of irreversibility in Fokker–Planck dynamics as related to the stochastic quantization procedure. We show in Section 3 that the Euler–Lagrange equations, *when interpreted at the c-number level*, have the remarkable property of being invariant under time-reversal as long as one assumes detailed balance in the form of the potential conditions.[34] This points to a quite unexpected relationship between the time-reversal invariance of the c-number Euler–Lagrange equations and the property of microscopic reversibility of which detailed balance is the expression.[34] Of course, this "semimicroscopic" reversibility of the Euler–Lagrange equations is broken once stochastic quantization is performed, leading to the well-known irreversibility associated with the FPE.

The work of Sections 2 and 3 is restricted to the case of constant diffusion coefficients. In Section 4 we consider the case of variable diffusion coefficients and show that this case can be reduced to that of constant diffusion by means of a transformation[35] whose significance has been discussed by Graham in the framework of a covariant formulation of the FPE.[36] This enables us to extend the results of Sections 2 and 3 to the case of variable diffusion as well.

Finally, we devote an appendix to discuss the relevance of our work to the stochastic formulation of quantum mechanics.[29–33] The latter formulation is shown to reduce to a "degenerate" FPE in which all sources of irreversibility cancel at all times.

2. PATH INTEGRAL FORMULATION AND STOCHASTIC QUANTIZATION

A continuous Markov process or "diffusion process"[37] describing the time evolution of a set of n gross variables $\{q_1,..., q_n\}$ is characterized by giving an expression for the transition probability density (conditional probability density) $\alpha(q, t; q', t')$ $(t > t')$. A particular process is then specified by a probability density $P(q_1,..., q_n; 0)$ for the state of the system under consideration at an initial time $t = 0$. For any other time $t > 0$, the state of the system is given by

$$P(q, t) = \int d^n q' \, \alpha(q, t; q', 0) P(q', 0) \tag{2.1}$$

We will consider here a continuous Markov process characterized by a transition probability expressed as a path integral in a phase space to be defined below. In the path integral, every path is differently weighted by the action integral, allowing for fluctuations around the most probable path. The most probable path in configuration space is defined by the Euler–Lagrange equations associated to the Lagrangian featuring in the path integral.[2] So, the path integral represents what we call here a "stochastic quantization" of such Euler–Lagrange equations.

[2] Although almost all paths of a diffusion process are nowhere differentiable, a sensible mathematical meaning can be given to a differentiable most probable tube of paths.[25,38] Such a most probable path is given by the usual Euler–Lagrange equations when the Lagrangian (2.2) is chosen.

Let us take as a starting point the Lagrangian[4,7,8,25–27]

$$\mathscr{L}(q, \dot{q}) = \tfrac{1}{4} D_{\mu\nu}^{-1}(\dot{q}_\mu - v_\mu)(\dot{q}_\nu - v_\nu) + \tfrac{1}{2}\, \partial v_\mu / \partial q_\mu \tag{2.2}$$

$D_{\mu\nu}$ is a symmetric, positive-definite, constant, real matrix and v_μ is a general real function of the gross variables q.

The canonical Hamiltonian associated to this Lagrangian is given by the following Legendre transformation:

$$p_\mu = \partial \mathscr{L}(q, \dot{q}) / \partial \dot{q}_\mu = \tfrac{1}{2} D_{\mu\nu}^{-1}(\dot{q}_\nu - v_\nu) \tag{2.3}$$

$$\mathscr{H}(q, p) = \dot{q}_\mu p_\mu - \mathscr{L} = D_{\mu\nu} p_\mu p_\nu + v_\mu p_\mu - \tfrac{1}{2}\, \partial v_\mu / \partial q_\mu \tag{2.4}$$

We now consider the analytical continuation of $\mathscr{H}(q, p)$ to the imaginary axis in the complex p plane. In other words, we consider (2.4) where p_μ is replaced by a pure imaginary variable. In terms of this analytical continuation of $\mathscr{H}(q, p)$ a continuous Markov process is defined by

$$\alpha(q, t; q', t') = \int \delta^n q(\tau)\, \delta^n p(\tau)\, e^{-A} \tag{2.5}$$

$$A = \int_{t'}^{t} [p_\mu(\tau) \dot{q}_\mu(\tau) - \mathscr{H}(q(\tau), p(\tau))]\, d\tau \tag{2.6}$$

where $q_\mu(\tau)$ is a real function and $p_\mu(\tau)$ a pure imaginary function.

The most probable path in (2.5) will be in general complex, and, as already pointed out by Phytian,[39] it lacks physical meaning. Nevertheless, if the p integration is carried out (which would not be possible for real p), only real paths survive in configuration space and they are weighted by $\exp\left[-\int_{t'}^{t'} \mathscr{L}(q(\tau), \dot{q}(\tau))\, d\tau\right]$, where $\mathscr{L}$ is the real-valued Lagrangian (2.2). This is the main difference between the problem at hand and a quantum problem with non-Hermitian Hamiltonian. In the quantum case the transition probability amplitude is a complex number and for a non-Hermitian Hamiltonian operator no real paths exist even in configuration space, since a complex Lagrangian is obtained. In our case, the path integral (2.5) defines a real transition probability and it can be understood as a "stochastic quantization" of the Euler–Lagrange equations associated with (2.2), which are equivalent to the Hamiltonian equations derived from the real-valued Hamiltonian (2.4).

We now derive from the path integral formulation (2.5)–(2.6) an equivalent operator formalism. We will show that the equation of motion of the operator formalism in the Schrödinger picture is a FPE for $P(q, t)$ with drift v_μ and diffusion $D_{\mu\nu}$. The equivalent Heisenberg picture equations of motion represent the so-called Fokker–Planck dynamics previously discussed by Garrido and San Miguel.[19,21] To the momentum p there corresponds an unobservable operator in the operator formalism. This unobservability can be understood as related to the imaginary character of p_μ in (2.5).

In order to accomplish this program a precise meaning has to be given to the phase-space path integral (2.5). In fact there exist a multiplicity of possible Lagrangians, each of which must be combined with an appropriate discretization of the path integral. The Lagrangian (2.2) corresponds to the so-called symmetric ordering[24] and this is the prescription adopted here for the path integral. Accordingly, we introduce[40] a network of $2N + 1$ times θ^i and we consider the action to depend on the values of p at time θ^{2i+1}, $i = 0,\ldots, N$, and the values of q at times θ^{2i}, $i = 1,\ldots, N$. The values of q and p are thus considered at alternating times on the network. We also require that the network becomes dense in such a way that the ratio of $\sum_{i=0}^{N} (\theta^{2i+2} - \theta^{2i+1})$ to $\sum_{i=0}^{N} (\theta^{2i+1} - \theta^{2i})$ tends to 1.

The path integral becomes

$$\alpha(q, t; q', t') = \lim_{N\to\infty} \int_{-\infty}^{\infty} \frac{1}{Z^{N+1}} \prod_{i=0}^{N} d^n p(\theta^{2i+1}) \prod_{i=1}^{N} d^n q(\theta^{2i}) e^{-A} \tag{2.7}$$

where

$$\begin{aligned} A = \sum_{i=0}^{N} \{ & p_\mu(\theta^{2i+1})[q_\mu(\theta^{2i+2}) - q_\mu(\theta^{2i})] \\ & - (\theta^{2i+2} - \theta^{2i+1})\mathscr{H}(q(\theta^{2i+2}), p(\theta^{2i+1})) \\ & - (\theta^{2i+1} - \theta^{2i})\mathscr{H}(q(\theta^{2i}), p(\theta^{2i+1}))\} \end{aligned} \tag{2.8}$$

Furthermore, one should take $\theta^0 = t$, $\theta^{2N+2} = t'$ and $q_\mu(t) = q_\mu$, $q_\mu(t') = q_\mu'$. The normalization constant $Z = (2\pi)^n i$ is fixed by the boundary condition

$$\alpha(q, t; q', t) = \delta^n(q - q') \tag{2.9}$$

The definition (2.7) of the path integral guarantees[40] the fulfillment of the Chapman–Kolomogorov equation[37]

$$\alpha(q, t; q', t') = \int d^n q^1\, \alpha(q, t; q^1, t^1)\alpha(q^1, t^1; q', t') \tag{2.10}$$

We now introduce operators $q_\mu^{\text{op}}(t^1)$ and $p_\mu^{\text{op}}(t^1)$ accounting for the possible alteration of a path by the appearance of dynamical variables at an intermediate time t_1:

$$\begin{aligned} q_\mu^{\text{op}}(t^1)\alpha(q, t; q', t') &= \int \delta^n q(\tau)\, \delta^n p(\tau)\, q_\mu(t^1) e^{-A} \\ &= \int d^n q^1\, \alpha(q, t; q^1, t^1) q_\mu(t^1) \alpha(q^1, t^1; q', t') \end{aligned} \tag{2.11}$$

$$\begin{aligned} p_\mu^{\text{op}}(t^1)\alpha(q, t; q', t') &= \int \delta^n q(\tau)\, \delta^n p(\tau)\, p_\mu(t^1) e^{-A} \\ d^n &\int = q^1\, \alpha(q, t; q^1, t^1) p_\mu(t^1) \alpha(q^1, t^1; q', t') \end{aligned} \tag{2.12}$$

where in the last equalities of Eqs. (2.11) and (2.12) use has been made of Eq. (2.10). If $t^1 = t$ or $t^1 = t'$ the action of $q_\mu^{\text{op}}(t^1)$ and $p_\mu^{\text{op}}(t^1)$ looks simpler. For $q_\mu^{\text{op}}(t^1)$ one has

$$q_\mu^{\text{op}}(t)\alpha(q, t; q', t') = q_\mu \alpha(q, t; q', t') \tag{2.13}$$

$$q_\mu^{\text{op}}(t')\alpha(q, t; q', t') = q_\mu{}'\alpha(q, t; q', t') \tag{2.14}$$

The action of $p_\mu^{\text{op}}(t^1)$ in these extreme time cases consists in the introduction in the integrand of the extreme values of p_μ, $p_\mu(\theta^{2N+1})$, and $p_\mu(\theta^1)$, respectively. This is achieved by taking derivatives of α with respect to q_μ and $q_\mu{}'$, respectively:

$$p_\mu^{\text{op}}(t)\alpha(q, t; q', t') = \hat{q}_\mu{}^+\alpha(q, t; q', t') \tag{2.15}$$

$$p_\mu^{\text{op}}(t')\alpha(q, t; q', t') = \hat{q}_\mu{}'\alpha(q, t; q', t') \tag{2.16}$$

Here we use the notation $\hat{q}_\mu = \partial/\partial q_\mu$, and $\hat{q}_\mu{}^+$ is the adjoint[21] of $\hat{q}_\mu$, i.e., $\hat{q}_\mu{}^+ = -\partial/\partial q_\mu$. Therefore, Eqs. (2.11) and (2.12) can be rewritten as

$$q_\mu^{\text{op}}(t^1)\alpha(q, t; q', t') = \int d^nq^1\, \alpha(q, t; q^1, t^1) q_\mu{}^1 \alpha(q^1, t^1; q', t') \tag{2.17}$$

$$\begin{aligned} p_\mu^{\text{op}}(t^1)\alpha(q, t; q', t') &= \int d^nq^1\, \alpha(q, t; q^1, t^1)\hat{q}_\mu^{1+}\alpha(q^1, t^1; q', t') \\ &= \int d^nq^1\, (\hat{q}_\mu{}^1\alpha(q, t; q^1, t^1))\alpha(q^1, t^1; q', t') \end{aligned} \tag{2.18}$$

On the same grounds it is possible to introduce time-ordered products of operators by

$$T(q_{\mu_1}^{\text{op}}(t^1) \cdots q_{\mu_l}^{\text{op}}(t^l) p_{\mu_{l+1}}^{\text{op}}(t^{l+1}) \cdots p_{\mu_m}^{\text{op}}(t^m))\alpha(q, t; q', t')$$

$$= \int \delta^n q(\tau)\, \delta^n p(\tau) q_{\mu_1}(t^1) \cdots q_{\mu_l}(t^l) p_{\mu_{l+1}}(t^{l+1}) \cdots p_{\mu_m}(t^m) e^{-A} \tag{2.19a}$$

$$\begin{aligned} &= \int d^nq^{\sigma_1} \cdots d^nq^{\sigma_m}\, \alpha(q, t; q^{\sigma_1}, t^{\sigma_1})\phi(t^{\sigma_1})\alpha(q^{\sigma_1}, t^{\sigma_1}; q^{\sigma_2}, t^{\sigma_2}) \cdots \phi(t^{\sigma_m}) \\ &\quad \times \alpha(q^{\sigma_m}, t^{\sigma_m}; q', t') \end{aligned} \tag{2.19b}$$

$$\begin{aligned} &= \int d^nq^{\sigma_1} \cdots d^nq^{\sigma_m}\, \alpha(q, t; q^{\sigma_1}, t^{\sigma_1})\Pi_1{}^+\alpha(q^{\sigma_1}, t^{\sigma_1}; q^{\sigma_2}, t^{\sigma_2}) \cdots \\ &\qquad \Pi_m{}^+\alpha(q^{\sigma_m}, t^{\sigma_m}; q', t') \\ &= \int d^nq^{\sigma_1} \cdots d^nq^{\sigma_m}(\Pi_1\alpha(q, t; q^{\sigma_1}, t^{\sigma_1})) \cdots (\Pi_m\alpha(q^{\sigma_{m-1}}, t^{\sigma_{m-1}}; q^{\sigma_m}, t^{\sigma_m})) \\ &\quad \times \alpha(q^{\sigma_m}, t^{\sigma_m}; q', t') \end{aligned} \tag{2.19c}$$

where we have used a specific notation:

$$T(q_{\mu_1}^{\text{op}}(t^1) \cdots p_{\mu_m}^{\text{op}}(t^m)) = \phi^{\text{op}}(t^{\sigma_1}) \cdots \phi^{\text{op}}(t^{\sigma_m}) \tag{2.20}$$

$\{t^{\sigma_1},\ldots, t^{\sigma_m}\}$ is the time-ordered permutation of $\{t^1,\ldots, t^m\}$, $\phi^{\mathrm{op}}(t^{\sigma_j})$ is the operator acting at t^{σ_j}, and $\phi(t^{\sigma_j})$ is the corresponding c-number dynamical variable. On the other hand, and according to (2.13)–(2.16),

$$\Pi_j = \begin{cases} q_{\mu_i}^{\sigma_j} & \text{if } \phi(t^{\sigma_j}) = q_{\mu_1}(t^{\sigma_j}) \\ \hat{q}_{\mu_i}^{\sigma_j} & \text{if } \phi(t^{\sigma_j}) = p_{\mu_1}(t^{\sigma_j}) \end{cases} \tag{2.21}$$

In the following we will need to consider the limits of Eq. (2.19) in which the intermediate times $\{t^1,\ldots, t^m\}$ tend to the extreme times t and t'. One can easily check from (2.19c) that

$$\lim_{t^{\sigma_m}\to \cdots \to t^{\sigma_1}\to t} T(q_{\mu_1}^{\mathrm{op}}(t^1)\cdots p_{\mu_m}^{\mathrm{op}}(t^m))\alpha(q, t; q', t') = \Pi_1{}^+ \cdots \Pi_m{}^+\alpha(q, t; q', t') \tag{2.22}$$

$$\lim_{t^{\sigma_1}\to \cdots \to t^{\sigma_m}\to t'} T(q_{\mu_1}^{\mathrm{op}}(t^1)\cdots p_{\mu_m}^{\mathrm{op}}(t^m))\alpha(q, t; q', t') = \Pi_m \cdots \Pi_1\alpha(q, t; q', t') \tag{2.23}$$

With the above definitions of operators it is now possible to derive the equations of motion satisfied by the transition probability $\alpha(q, t; q', t')$. From eqs. (2.5) and (2.6)

$$\frac{\partial\alpha(q, t; q', t')}{\partial t} = \int \delta^n q(\tau)\, \delta^n p(\tau) \left(\frac{\partial}{\partial t}\int_{t'}^{t} \mathscr{H}\, d\tau\right) e^{-A} \tag{2.24}$$

The derivative of the time integral of the Hamiltonian is obtained by continuing the integral for a time Δt, extending the network used in the definition of the path integral,[40] i.e.,

$$\frac{\partial}{\partial t}\int_{t'}^{t} \mathscr{H}\, d\tau = \lim_{\Delta t\to 0} \frac{\int_t^{t+\Delta t} \mathscr{H}\, d\tau}{\Delta t} \tag{2.25}$$

Dividing Δt by means of a network of $2N' + 1$ times with $(\theta')^0 = t$ and $(\theta')^{2N'+2} = t + \Delta t$, in the limit $\Delta t \to 0$, $N' \to \infty$, one obtains that due to the requirement on the way in which the network becomes dense,

$$\frac{\partial}{\partial t}\int_{t'}^{t} \mathscr{H}\, d\tau = \lim_{\delta\to 0} \frac{1}{2}\, [\mathscr{H}(q(\tau), p(\tau - \delta)) + \mathscr{H}(q(\tau - \delta), p(\tau))] \tag{2.26}$$

Substituting (2.26) into (2.24) and recalling (2.19a), we obtain

$$(\partial/\partial t)\alpha(q, t; q', t') = \lim_{\delta\to 0} \tfrac{1}{2} T(\mathscr{H}(q^{\mathrm{op}}(t), p^{\mathrm{op}}(t - \delta)) + \mathscr{H}(q^{\mathrm{op}}(t - \delta), p^{\mathrm{op}}(t)))\alpha(q, t; q', t') \tag{2.27}$$

Taking the limit according to (2.22) and the explicit form of the Hamiltonian function (2.4) yields

$$(\partial/\partial t)\alpha(q, t; q', t') = (\hat{q}_\mu{}^+\hat{q}_\nu{}^+ D_{\mu\nu} + \hat{q}_\mu{}^+ v_\mu)\alpha(q, t; q', t') = L^+(q, \hat{q})\alpha(q, t; q', t') \tag{2.28}$$

where we have defined by the last equality the Fokker–Planck operator or adjoint Fokker–Planck Liouvillian[21] $L^+(q, \hat{q})$. This equation of motion is known as the forward FPE for the transition probability.[37]

By the same procedure the equation of motion of $\alpha(q, t; q', t')$ with respect to t' is obtained:

$$\frac{\partial \alpha(q, t; q', t')}{\partial t'} = \int \delta^n q(\tau)\, \delta^n p(\tau) \left(\lim_{\Delta t' \to 0} - \frac{\int_{t'-\Delta t'}^{t'} \mathscr{H}\, d\tau}{\Delta t'} \right) e^{-A}$$
$$= -\lim_{\delta \to 0} \tfrac{1}{2} T(\mathscr{H}(q^{\mathrm{op}}(t' + \delta), p^{\mathrm{op}}(t')) + \mathscr{H}(q^{\mathrm{op}}(t'), p^{\mathrm{op}}(t' + \delta)))\alpha(q, t; q', t') \tag{2.29}$$

The limit to be considered now is (2.23) and it yields

$$\begin{aligned} \partial\alpha(q, t; q', t')/\partial t' &= -(D_{\mu\nu}\hat{q}_\mu\hat{q}_\nu + v_\mu\hat{q}_\mu)\alpha(q, t; q', t') \\ &= -L(q, \hat{q})\alpha(q, t; q', t') \end{aligned} \tag{2.30}$$

This equation of motion complementary to (2.28) is known as the backward FPE[37] and L is the adjoint of the Fokker–Planck operator or Fokker–Planck Liouvillian.[21]

It should be remarked that both forward and backward FPEs have been deduced from the path integral definition of $\alpha(q, t; q't')$, and that the derivation depends crucially on the presence of the term $\frac{1}{2}\, \partial v_\mu/\partial q_\mu$ in the Lagrangian and on the definition of the path integral.

The equations of motion for the operators $q_\mu^{\mathrm{op}}(t^1)$ and $p_\mu^{\mathrm{op}}(t^1)$ can be obtained from their definitions (2.17) and (2.18) and from (2.28) and (2.30). For example, taking the derivative of (2.18) with respect to t_1, we obtain

$$\begin{aligned} &\frac{\partial p_\mu^{\mathrm{op}}(t^1)}{\partial t^1}\, \alpha(q, t; q', t') \\ &\quad = \int d^n q^1\, (-L(q^1, \hat{q}^1)\alpha(q, t; q^1, t^1))\hat{q}_\mu^{1+}\alpha(q^1, t^1; q', t') \\ &\quad\quad + \int d^n q^1\, \alpha(q, t; q^1, t^1)\hat{q}_\mu^{1+} L^+(q^1, \hat{q}^1)\alpha(q^1, t^1; q', t') \\ &\quad = \int d^n q^1\, \alpha(q, t; q^1, t^1)[\hat{q}_\mu^{1+}, L^+(q^1, \hat{q}^1)]\alpha(q^1, t^1; q', t') \end{aligned} \tag{2.31}$$

and therefore

$$\partial p_\mu^{\mathrm{op}}(t^1)/\partial t^1 = [p_\mu^{\mathrm{op}}(t^1), H_{\mathrm{op}}(t^1)] \tag{2.32}$$

where[3]

$$H_{\mathrm{op}}(t^1) = \lim_{\delta \to 0} \tfrac{1}{2} T(\mathscr{H}(q^{\mathrm{op}}(t^1), p^{\mathrm{op}}(t^1 - \delta)) + \mathscr{H}(q^{\mathrm{op}}(t^1 - \delta), p^{\mathrm{op}}(t^1))) \tag{2.33}$$

[3] Equation (2.33) represents the symmetric or Weyl correspondence rule[41] (they coincide in our case of constant diffusion).

The precise meaning of the right-hand side of (2.32) is a limit of a time-ordered product of operators whose action, defined by (2.19), yields Eq. (2.31), i.e.,

$$[p_\mu^{\rm op}(t^1), H_{\rm op}(t^1)] \equiv \lim_{\delta' \to 0} T(p_\mu^{\rm op}(t^1 + \delta')H_{\rm op}(t^1) - p_\mu^{\rm op}(t^1 - \delta')H_{\rm op}(t^1)) \quad (2.34)$$

On the same grounds the equation of motion for $q_\mu^{\rm op}(t^1)$ is

$$\partial q_\mu^{\rm op}(t^1)/\partial t^1 = [q_\mu^{\rm op}(t^1), H_{\rm op}(t^1)] \quad (2.35)$$

It is thus established that $H_{\rm op}$ generates the motion of the operators and of the transition probability.

To this point the formalism developed is closely related to the derivation of the Schrödinger–Heisenberg formulation of quantum mechanics from Feynman's formulation. Nevertheless, a striking difference has to be remarked: although a bracket notation for $\alpha(qt; q't')$ could sometimes be useful,(14) the transition probability is a real number, while the quantum mechanical bracket is a complex probability amplitude and thus $\alpha(qt; q't')$ cannot be interpreted as the product of a vector of a Hilbert space times a vector of the dual of the same Hilbert space. In other words, initial and final states are not related here by a complex conjugation. This is the reason why the explicit form at different times of a uniquely defined operator is different: the content of Eqs. (2.15) and (2.16) is different, while the analogous quantum mechanical equations are related by complex conjugation (even for a non-Hermitian Hamiltonian). The action of $H_{\rm op}(t^1)$ on a final time yields the forward FPE and its action on an initial time yields the backward FPE. The analogous equations in quantum mechanics are again related by complex conjugation. This asymmetry between initial and final states forces us to give some specification to obtain from (2.32) and (2.35) the operator equations of motion in a Heisenberg picture.

The state of the system is described by $P(q, t)$. From Eq. (2.1) it is clear that the arguments of $P(q, t)$ represent a final state. Indeed, Eq. (2.28) implies that $P(q, t)$ satisfies the FPE

$$\frac{\partial P(q,t)}{\partial t} = L^+(q, \hat{q})P(q,t) = -\frac{\partial}{\partial q_\mu}[v_\mu(q)P(q,t)] + \frac{\partial^2}{\partial q_\mu \partial q_\nu} D_{\mu\nu}P(q,t) \quad (2.36)$$

We note that no backward FPE exists for $P(q, t)$.

The FPE (2.36) is an equation of motion for the state of the system and it defines the Schrödinger picture. In this picture $H_{\rm op}(t)$ acts explicitly as $L^+(q, \hat{q})$ and the average of a function of q at time t is evaluated by

$$\langle f(q(t))\rangle = \int d^n q\, P(q,t) f(q) \quad (2.37)$$

In the corresponding adjoint picture (Heisenberg picture) the time evolution is transferred to the dynamical variables. The two possible specifications of (2.32) and (2.35) that follow from (2.22) and (2.23) give rise to operator equations related by the adjoint operation and the choice of one of them is forced by the prescription one gives to evaluate average quantities. Our prescription is the one contained in the so-called Fokker–Planck dynamics, in which, as discussed at length in Ref. 21, averages are evaluated with the initial probability density $P(q, 0)$ placed at the left of the dynamical variables, which behave as operators acting on their initial values. For such a prescription, the initial time specification of (2.32) and (2.35) must be chosen. This assertion can be better understood rewriting (2.37) as

$$\begin{aligned}\langle f(q(t))\rangle &= \int d^nq\,[e^{L^+t}P(q,0)]f(q)\\ &= \int d^nq\,P(q,0)e^{Lt}f(q) = \int d^nq\,P(q,0)f(q(t)) \qquad (2.38)\end{aligned}$$

It is then clear that L generates the motion of $q(t)$ with initial value $q(0) = q$.

Summarizing, in this Heisenberg picture, the explicit forms of $[q_\mu^{\mathrm{op}}(t), H_{\mathrm{op}}(t)]$ and $[p_\mu^{\mathrm{op}}(t), H_{\mathrm{op}}(t)]$ appearing in Eqs. (2.32) and (2.35) are, respectively, $[L(q(t), \hat{q}(t)), q_\mu(t)]$ and $[L(q(t), q(t)), \hat{q}_\mu(t)]$ as results from (2.14), (2.16), (2.23), and (2.33). In conclusion, the stochastic quantization of the Hamiltonian equations corresponding to the c-number real Hamiltonian (2.4), which are equivalent to the Euler–Lagrange equations associated to (2.2), is given by

$$\begin{aligned}q_\mu(t) &\to q_\mu(t)\\ p_\mu(t) &\to \hat{q}_\mu(t)\\ \mathscr{H}(q(t), p(t)) &\to -L(q(t), \hat{q}(t))\end{aligned}$$

so that the commutation relations at equal times are

$$[\hat{q}_\mu(t), q_\nu(t)] = \delta_{\mu\nu} \qquad (2.39)$$

and the equations of motion[21]

$$\dot{q}_\mu(t) = [L(q(t), \hat{q}(t)), q_\mu(t)] = v_\mu(q(t)) + 2D_{\mu\nu}\hat{q}_\nu(t) \qquad (2.40)$$

$$\dot{\hat{q}}_\mu(t) = [L(q(t), \hat{q}(t)), \hat{q}_\mu(t)] = -\frac{\partial v_\nu(q(t))}{\partial q_\mu(t)}\,\hat{q}_\nu(t) \qquad (2.41)$$

The key implication of these equations is the lack of commutativity of the gross variables $q_\mu(t)$ at different times, which reflects the stochastic character of the process.[21] The formal solution of (2.40) reads

$$q_\mu(t) = e^{Lt}q_\mu(0)e^{-Lt} \qquad (2.42)$$

The factor e^{-Lt} is of crucial importance when evaluating correlation functions of q variables at different times in specific problems.[42] Nevertheless, when placed at the extreme right of an integral, as it appears in one-time averages, it can be suppressed, since it acts on unity, giving value one. This is why the last equality in (2.38) is in agreement with (2.42).

On the other hand, the solution of (2.40)–(2.41) gives $\hat{q}_\mu(t)$ in terms of its initial values $\hat{q}_\mu(0)$, so that $\hat{q}_\mu(t)$ is an operator which derives with respect to the initial values of $q_\mu(t)$, i.e., $q_\mu(0) = q_\mu$. The operator $\hat{q}_\mu(t)$ is unobservable but is very useful to define response functions.[21]

Finally we note that Eq. (2.41) is not formally equal to the c-number Hamilton equation for $p_\mu(t)$, due to the disappearance in L of the $-\frac{1}{2}\,\partial v_\mu/\partial q_\mu$ term of $\mathscr{H}$ that occurs in the stochastic quantization procedure. This point clarifies earlier results by Phytian,[39] who only considers c-number equations.

3. IRREVERSIBILITY

The irreversibility of the Fokker–Planck equation is reflected in the fact that (2.36) is not invariant under the time-reversal operation

$$\begin{gathered} t \to -t, \qquad q_\mu \to q_\mu \\ v_\mu{}^R \to -v_\mu{}^R, \qquad v_\mu{}^I \to v_\mu{}^I, \qquad D_{\mu\nu} \to D_{\mu\nu} \end{gathered} \tag{3.1}$$

where without loss of generality, we may assume that the gross variables q_μ are even under time reversal and where $v_\mu{}^R$ and $v_\mu{}^I$ are, respectively, the reversible and irreversible parts of the drift.[4] Note that the reversible part $v_\mu{}^R$ transforms as $\dot{q}_\mu$ and that there are two sources of irreversibility in the FPE: the irreversible drift $v_\mu{}^I$ and the diffusion coefficients $D_{\mu\nu}$. An irreversible behavior in the sense of dissipation is affected by the diffusion. This should not be confused with the irreversibility in the sense of a deterministic but not time-reversal invariant equation of motion as $\dot{q}_\mu = v_\mu{}^I$. Under the very special conditions in which these two terms featuring the irreversible drift $v_\mu{}^I$ and the diffusion coefficient $D_{\mu\nu}$ cancel one another, the FPE becomes time-reversal invariant. This is the case in stochastic models of quantum mechanics[29–33] (see appendix). It should also be stressed that the time-reversed Fokker–Planck operator

$$\hat{q}_\mu{}^+(v_\mu{}^R - v_\mu{}^I) + \hat{q}_\mu{}^+\hat{q}_\nu{}^+ D_{\mu\nu} \tag{3.2}$$

is different from the adjoint operator $L(q, \hat{q})$

$$(v_\mu{}^R + v_\mu{}^I)\hat{q}_\mu + D_{\mu\nu}\hat{q}_\mu\hat{q}_\nu \tag{3.3}$$

which appears in the backward FPE (2.30).[43]

[4] If all gross variables are even under time reversal, then a reversible drift can arise only from a dependence of v_μ on some external parameters which change sign under time reversal. We shall not indicate dependence on these variables explicitly.

How does irreversibility manifest itself in the stochastic quantization scheme? Consider the simplest example of one-dimensional, constant diffusion and linear irreversible drift with $v^R = 0$.[1] The corresponding Lagrangian is

$$\mathscr{L}(q, \dot{q}) = \frac{1}{4D}(\dot{q} + \alpha q)^2 - \frac{\alpha}{2} \tag{3.4}$$

and the Euler–Lagrange equation

$$\ddot{q} - \alpha^2 q = 0 \tag{3.5}$$

is invariant under time reversal. However, the Lagrangian is not and, as was already noted by Onsager and Machlup,[1] the two independent solutions $q \sim e^{-\alpha t}$ and $q \sim e^{+\alpha t}$ give different contributions to the path integral due to the irreversibility of $\mathscr{L}$. It is also easy to see that stochastic quantization for this example leads to operator equations of motion and commutation relations which break the time-reversal symmetry of the Euler–Lagrange equation. What we shall now show is that this holds true in general as long as the detailed balance conditions[34] are satisfied. This general connection between detailed balance and time-reversal invariance of the Euler–Lagrange equations is rather unexpected. Although one knows that detailed balance is an expression of microscopic reversibility,[34] the connection between the latter and the time-reversal invariance of the Euler–Lagrange equations for the gross variables is far from evident. In this section we shall consider the case of general drift in n dimensions but with constant diffusion matrix. Consideration of the variable-diffusion case is deferred to Section 4.

The Lagrangian (2.2) yields the Euler–Lagrange equations

$$\ddot{q}_\mu - \frac{\partial v_\mu}{\partial q_\nu}\dot{q}_\nu + D_{\mu\delta}D^{-1}_{\beta\nu}\frac{\partial v_\beta}{\partial q_\delta}(\dot{q}_\nu - v_\nu) - D_{\mu\delta}\frac{\partial^2 v_\beta}{\partial q_\delta\, \partial q_\beta} = 0 \tag{3.6}$$

Equation (3.6) is invariant under time reversal if the following condition is fulfilled:

$$\left(-\frac{\partial v_\mu{}^I}{\partial q_\nu} + D_{\mu\delta}D^{-1}_{\beta\nu}\frac{\partial v_\beta{}^I}{\partial q_\delta}\right)\dot{q}_\nu - D_{\mu\delta}D^{-1}_{\beta\nu}\left(\frac{\partial v_\beta{}^R}{\partial q_\delta}v_\nu{}^I + \frac{\partial v_\beta{}^I}{\partial q_\delta}v_\nu{}^R\right)$$
$$- D_{\mu\delta}\frac{\partial^2 v_\beta{}^R}{\partial q_\delta\, \partial q_\beta} = 0 \tag{3.7}$$

On the other hand, the Graham–Haken potential conditions, which follow from the assumption of detailed balance, are[34]

$$v_\mu{}^I = -D_{\mu\nu}\, \partial\phi_{\text{st}}/\partial q_\nu \tag{3.8}$$

$$\partial v_\mu{}^R/\partial q_\mu = v_\mu{}^R\, \partial\phi_{\text{st}}/\partial q_\mu \tag{3.9}$$

where ϕ_{st} is the "potential function" defined in terms of the stationary solution $P_{st}(q)$ of the FPE by

$$\phi_{st}(q) = -\log P_{st}(q) \tag{3.10}$$

It is a straightforward calculation to show that the potential conditions (3.8) and (3.9) ensure that condition (3.7) is fulfilled, thereby guaranteeing the reversibility of the Euler–Lagrange equations (3.6). An important point to note is that the presence of the $\frac{1}{2}\,\partial v_\mu/\partial q_\mu$ term in the Lagrangian is essential for this to be true.[5]

Although the Euler–Lagrange equations are time-reversal invariant, the Lagrangian (2.2) itself is not. Under time reversal $\mathscr{L}$ transforms into $\mathscr{L}'$ given by

$$\mathscr{L}'(q,\dot{q}) = \tfrac{1}{4}D_{\mu\nu}^{-1}(-\dot{q}_\mu + v_\mu{}^R - v_\mu{}^I)(-\dot{q}_\nu + v_\nu{}^R - v_\nu{}^I) - \frac{1}{2}\frac{\partial v_\mu{}^R}{\partial q_\mu} + \frac{1}{2}\frac{\partial v_\mu{}^I}{\partial q_\mu} \tag{3.11}$$

As mentioned earlier in connection with the simple example (3.4), a time-reversal-invariant Lagrangian would not be compatible with overall irreversibility in the path integral formulation of Fokker–Planck dynamics. However, a time-reversal invariant Lagrangian yielding (3.6) as its Euler–Lagrange equations does exist: it is

$$\mathscr{L}^{\text{inv}}(q,\dot{q}) = \tfrac{1}{4}D_{\mu\nu}^{-1}[(\dot{q}_\mu - v_\mu{}^R)(\dot{q}_\nu - v_\nu{}^R) + v_\mu{}^I v_\nu{}^I] + \tfrac{1}{2}\,\partial v_\mu{}^I/\partial q_\mu \tag{3.12}$$

Assuming again that detailed balance holds [Eqs. (3.8) and (3.9)], one easily finds

$$\mathscr{L} - \mathscr{L}^{\text{inv}} = \frac{1}{2}\frac{\partial \phi_{st}}{\partial q_\mu}\dot{q}_\mu = \frac{1}{2}\frac{d\phi_{st}}{dt} \tag{3.13}$$

Equation (3.13) exhibits $\mathscr{L}$ as the sum of two terms: $\mathscr{L}^{\text{inv}}$, which is even under time reversal, and an odd term $\frac{1}{2}\,d\phi_{st}/dt$ which, when inserted into the path integral weight function $\exp\left(-\int \mathscr{L}\,d\tau\right)$, yields a term dependent only on the initial and final times. This decomposition of $\mathscr{L}$ gives an insight into its interpretation as a thermodynamical potential.[8] In the particular case of linear drift the term "thermodynamic action" has been applied by Lavenda[11] to the integral $\int \mathscr{L}^{\text{inv}}\,d\tau$. The physical interpretation of the $d\phi_{st}/dt$ term is the subject of considerable controversy.[44,45] It seems doubtful whether ϕ_{st} can be consistently identified with physical entropy as claimed by Lavenda[11]

[5] In a related result previously obtained by Ueyama[6] this important surface term was neglected. Moreover, Ueyama makes an additional assumption [his Eq. (25)] whose meaning is unclear and which, he erroneously claims, follows from the potential conditions. Hasegawa stated the above result in Ref. 43.

and also by Ueyama.[6] It is also worth noting that the decomposition (3.13) has been used for the explicit construction of $\mathscr{L}$ in the case in which $v_\mu{}^R = 0$.[46,26,12] Detailed balance and this further condition are always satisfied in one-dimensional problems[26,12] if natural boundary conditions are considered. The term

$$\mathscr{L}^{\text{inv}} = \tfrac{1}{4} D_{\mu\nu}^{-1} v_\mu{}^I v_\nu{}^I + \tfrac{1}{2}\, \partial v_\mu{}^I / \partial q_\mu$$

represents then the mechanical potential of the self-adjoint form of the FPE and $e^{-\phi_{\text{st}}/2}$ is the factor coming from the transformation to this self-adjoint form.

In contrast to the noninvariance of the Lagrangian, the real Hamiltonian (2.4) is time-reversal invariant, provided detailed balance is satisfied. This follows from the transformation

$$p_\mu \to -p_\mu - D_{\mu\nu}^{-1} v_\nu{}^I \tag{3.14}$$

which is in turn a consequence of the definition (2.3) of p and the transformation (3.1). Of course, the c-number real Hamilton equations of motion are also time-reversal invariant under the same conditions.

The operator formulation of stochastic quantization, as we have seen in Section 2, is based upon two mutually consistent sets of premises: (a) equal-time commutation relations [Eq. (2.39)], and (b) equations of motion of the form (2.40) and (2.41). While detailed balance ensures the time-reversal invariance of the Euler–Lagrange equations (3.6) at the c-number level, this invariance cannot be extended to the stochastic quantized level. Stated differently, stochastic quantization breaks the time-reversal symmetry of the equations of motion. The problem lies in the incompatibility between the condition for time-reversal invariance of the equations of motion and the corresponding condition for the invariance of the commutation relations. If $\hat{q}_\mu$ transforms as p_μ in (3.14), the equation for q_μ, (2.40), is invariant, but the commutation relations are not time-reversal invariant. Under this transformation the equation for $\hat{q}_\mu$, (2.41), is not in general invariant, but the important point is the breaking of the time-reversal invariance of the commutation relations, as can be easily realized considering the special case of linear drift $v_\mu = A_{\mu\nu} q_\nu$. In this case, the $-\frac{1}{2}\, \partial v_\mu / \partial q_\mu$ term in the Hamiltonian (2.4) is just a constant and so the c-number real Hamilton equations are formally identical to the operator equations (2.40) and (2.41). Both equations (2.40) and (2.41) are then invariant, but the commutation relations are not. On the other hand, the identification $\hat{q}_\mu = \partial / \partial q_\mu$ requires the transformation law $\hat{q}_\mu \to \hat{q}_\mu$, in which case the commutation relations are invariant but the equations of motion become noninvariant.

In conclusion, stochastic quantization introduces some uncertainty or loss of determinism with respect to the Euler–Lagrange equations defining the most probable path, which causes an irreversible behavior. In the path integral formulation of the stochastic quantization, irreversibility is due to the Lagrangian itself, while in the equivalent operator formalism it appears as a requirement of consistency between equations of motion and commutation relations.

4. NONCONSTANT DIFFUSION FPE

In this section we show how the FPE

$$\frac{\partial P(q,t)}{\partial t} = -\frac{\partial}{\partial q_\mu}[v_\mu P(q,t)] + \frac{\partial^2}{\partial q_\mu\,\partial q_\nu}[D_{\mu\nu}(q)P(q,t)] \tag{4.1}$$

with nonconstant diffusion coefficients $D_{\mu\nu}(q)$ can be reduced to one with constant diffusion coefficients by means of a change of variables.[35,27] This result generalizes previous work for the one-dimensional case[4,26,47] and its significance has been discussed in detail by Graham[36]: in a covariant formulation of the FPE it represents a transformation to a set of holonomous coordinates. The possibility of performing this kind of reduction eliminates, in such a case, the need for a separate discussion of the nonconstant diffusion case. Instead the results of Sections 2 and 3 may be applied directly to the constant-diffusion FPE in the transformed variables, as we shall show.

The diffusion matrix $D_{\mu\nu}(q)$ is a symmetric, positive-definite, $n \times n$ matrix, and therefore there exists[3,48] a real, symmetric, $n \times n$ matrix $g_{\mu\nu}(q)$ such that

$$g_{\mu\alpha}(q)g_{\alpha\nu}(q) = D_{\mu\nu}(q) \tag{4.2}$$

Let us introduce a new set of n gross variables Q_μ by

$$dQ_\mu = g_{\mu\nu}^{-1}\,dq_\nu \tag{4.3}$$

The condition for the Q_μ to be well defined is that dQ_μ be an exact differential, i.e., that

$$\frac{\partial g_{\alpha\mu}^{-1}}{\partial q_\nu} - \frac{\partial g_{\alpha\nu}^{-1}}{\partial q_\mu} = 0 \tag{4.4}$$

Graham[36] has called (4.4) a "holonomity condition" in his covariant formulation of the FPE. Such a condition implies that $D_{\mu\nu}(q)$ can be considered as a Euclidean metric and therefore there exists a set of coordinates in which $D_{\mu\nu} = \delta_{\mu\nu}$. We will now show explicitly that indeed in the FPE in the Q variables the diffusion matrix is $\delta_{\mu\nu}$.

Condition (4.4) implies that

$$\frac{1}{2}\frac{D_{\mu\nu}}{D}\frac{\partial D}{\partial q_\mu} = \frac{\partial g_{\mu\alpha}}{\partial q_\mu} g_{\alpha\nu} \tag{4.5}$$

where $D = \|D_{\mu\nu}\|$ is the determinant of the $D_{\mu\nu}$ matrix. It is in this form that we shall use the holonomity condition throughout the remainder of this paper.

Denoting $P(q(Q), t)$ by $\mathscr{P}(Q, t)$, we have

$$\langle f(q(t))\rangle = \int d^n q\, P(q, t) f(q) = \int d^n Q \left| \left\| \frac{\partial q_\mu}{\partial Q_\nu} \right\| \right| \mathscr{P}(Q, t) f(q(Q)) \tag{4.6}$$

so that the Fokker–Planck distribution function in the Q variables is

$$P'(Q, t) = \mathscr{P}(Q, t)\sqrt{D} \tag{4.7}$$

Derivation of the corresponding FPE in the new variables is somewhat lengthy. Summarizing the main steps in the calculation, the substitution of (4.7) into (4.1) and use of (4.3) yields

$$\begin{aligned} \frac{\partial P'(Q, t)}{\partial t} &= -\sqrt{D}\, g_{\nu\mu}^{-1} \frac{\partial}{\partial Q_\nu} \frac{v_\mu}{\sqrt{D}} P'(Q, t) \\ &\quad + \sqrt{D}\, g_{\alpha\mu}^{-1} \frac{\partial}{\partial Q_\alpha} g_{\beta\nu}^{-1} \frac{\partial}{\partial Q_\beta} \frac{D_{\mu\nu}}{\sqrt{D}} P'(Q, t) \end{aligned} \tag{4.8}$$

The condition (4.5) implies, when (4.3) is used, that

$$[\hat{Q}_\nu, \sqrt{D}\, g_{\nu\mu}^{-1}] = 0 \tag{4.9}$$

By means of (4.9) the first term on the right-hand side of (4.8) reduces to $-(\partial/\partial Q_\mu) g_{\mu\nu}^{-1} v_\nu P'$. The second term is simplified in two steps. In a first step $\partial/\partial Q_\alpha$ is written in the extreme left using (4.9). In a second step $\partial/\partial Q_\beta$ is taken to act directly on $P'(q, t)$ and the commutator involved is simplified according to (4.5). Finally, we obtain that

$$\begin{aligned} \frac{\partial P'(Q, t)}{\partial t} &= -\frac{\partial}{\partial Q_\mu} g_{\mu\nu}^{-1} v_\nu P'(Q, t) \\ &\quad + \frac{\partial}{\partial Q_\mu} g_{\alpha\mu}^{-1} \frac{\partial g_{\beta\alpha}}{\partial Q_\beta} P'(Q, t) + \frac{\partial^2}{\partial Q_\mu{}^2} P'(Q, t) \\ &= -\frac{\partial}{\partial Q_\mu} [v_\mu' P'(Q, t)] + \frac{\partial^2}{\partial Q_\mu{}^2} P'(Q, t) \end{aligned} \tag{4.10}$$

where the last equality defines the transformed drift $v_\mu'(Q)$ and where it is verified that $\delta_{\mu\nu}$ appears as the diffusion matrix for the FPE in the Q variables.[6]

It was shown in Section 2 that we can associate to the FPE (4.10) a Lagrangian

$$\mathscr{L}(Q, \dot{Q}) = \tfrac{1}{4}(\dot{Q}_\mu - v_\mu')^2 + \tfrac{1}{2}\, \partial v_\mu'/\partial Q_\mu \tag{4.11}$$

which under stochastic quantization yields as generator of motion the operator

$$L(Q, \hat{Q}) = \hat{Q}_\mu \hat{Q}_\mu + v_\mu'(Q)\hat{Q}_\mu \tag{4.12}$$

The generator of motion for the Fokker–Planck dynamics associated to our starting FPE (4.1) is now obtained by reexpressing L given by (4.12) in terms of q_μ and $\hat{q}_\mu$ through the use of (4.3):

$$\begin{aligned} L(q, \hat{q}) &= g_{\mu\alpha}(q)\hat{q}_\alpha g_{\mu\beta}(q)\hat{q}_\beta + \left[v_\mu(q) - g_{\beta\nu}(q)\,\frac{\partial g_{\beta\mu}(q)}{\partial q_\nu(q)}\right]\hat{q}_\mu \\ &= D_{\mu\nu}(q)\hat{q}_\mu\hat{q}_\nu + v_\mu(q)\hat{q}_\mu \end{aligned} \tag{4.13}$$

Obviously, the Liouvillian obtained is the adjoint of the Fokker–Planck operator featured in (4.1).

The results of Section 3 may be now applied directly to the Lagrangian (4.11) and to its stochastic quantization. The key assumption made in that section was the fulfillment of the potential conditions (3.8) and (3.9). Thus, the discussion of the time-reversal properties made in Section 3 and its application to (4.11) will be meaningful for the FPE (4.1) whenever potential conditions for (4.10) could be deduced from the potential conditions for (4.1). We now show that this is the case for the transformation (4.3). Detailed balance is assumed for the starting FPE (4.1) and the corresponding potential conditions are[34]

$$v_\mu{}^I(q) = \frac{\partial D_{\mu\nu}(q)}{\partial q_\nu} - D_{\mu\nu}\,\frac{\partial \phi_{\text{st}}(q)}{\partial q_\nu} \tag{4.14}$$

$$\frac{\partial v_\mu{}^R(q)}{\partial q_\mu} = v_\mu{}^R(q)\,\frac{\partial \phi_{\text{st}}(q)}{\partial q_\mu}$$

where

$$\phi_{\text{st}}(q) = -\log P_{\text{st}}(q) \tag{4.16}$$

The definition (4.10) of v_μ' implies that

$$v_\mu'^R(Q) = g_{\mu\nu}^{-1}(Q)v_\nu{}^R \tag{4.17}$$

$$v_\mu'^I(Q) = g_{\mu\nu}^{-1}(Q)v_\nu{}^I - g_{\alpha\mu}^{-1}(Q)\,\partial g_{\beta\alpha}(Q)/\partial Q_\beta \tag{4.18}$$

[6] It is interesting to mention that the inverse transformation from (4.10) to (4.1) allows one to consider a class of exactly solvable nonlinear FPEs.[49]

From Eq. (4.17) and substituting (4.15),

$$\frac{\partial v_\mu'^R(Q)}{\partial Q_\mu} = v_\alpha'^R(Q)\frac{\partial\phi_{st}(q(Q))}{\partial Q_\alpha} + g_{\nu\alpha}(Q)v_\alpha'^R(Q)\frac{\partial g_{\mu\alpha}^{-1}(Q)}{\partial Q_\mu}$$

$$= v_\alpha'^R(Q)\frac{\partial}{\partial Q_\alpha}[\phi_{st}(q(Q)) - \log\sqrt{D}] \tag{4.19}$$

where in the last equality use has been made of (4.5) expressed in Q variables. Substituting (4.18) in (4.14) and using (4.5) again, one easily arrives at

$$v_\mu'^I(Q) = -(\partial/\partial Q_\mu)[\phi_{st}(q(Q) - \log\sqrt{D})] \tag{4.20}$$

Equations (4.19) and (4.20) are recognized as the potential conditions for the FPE (4.10) [see (3.8) and (3.9)] because

$$\phi_{st}'(Q) \equiv -\log P_{st}'(Q) = -\log[P_{st}(q(Q))\sqrt{D}] = \phi_{st}(q(Q)) - \log\sqrt{D} \tag{4.21}$$

The reason for this conservation of the potential conditions under the change of coordinates (4.3) is basically found in Graham's formulation[36] of detailed balance as a covariant physical property.

It is finally instructive to look at the properties of the Lagrangian (4.11) when expressed in terms of q variables by means of the point canonical transformation (4.3). Defining w_μ by

$$v_\mu' = g_{\mu\nu}^{-1}w_\nu \tag{4.22}$$

and taking into account that

$$\dot{Q}_\mu = (\partial Q_\mu/\partial q_\nu)\dot{q}_\nu = g_{\mu\nu}^{-1}\dot{q}_\nu \tag{4.23}$$

we can write the Lagrangian (4.11) as

$$\mathscr{L}(q,\dot{q}) = \frac{1}{4}[g_{\mu\nu}^{-1}(\dot{q}_\nu - w_\nu)]^2 + \frac{1}{2}g_{\mu\nu}\frac{\partial}{\partial q_\nu}(g_{\mu\alpha}^{-1}w_\alpha)$$

$$= \frac{1}{4}D_{\mu\nu}^{-1}(\dot{q}_\mu - w_\mu)(\dot{q}_\nu - w_\nu) + \frac{1}{2}\sqrt{D}\frac{\partial}{\partial q_\mu}\frac{w_\mu}{\sqrt{D}} \tag{4.24}$$

where to obtain the last equality the holonomity condition (4.5) is used. It should be remarked that (4.24) coincides with the Lagrangian already proposed by Stratonovich and Graham for flat spaces.[8] This coincidence is established at once since (4.5) yields the following explicit expression for w_μ:

$$w_\mu = v_\mu - \sqrt{D}\frac{\partial}{\partial q_\nu}\frac{D_{\mu\nu}}{\sqrt{D}} \tag{4.25}$$

The restriction to flat spaces has been introduced here through the holonomity condition (4.4).

The fact that Eq. (4.24) coincides with the Graham–Stratonovich Lagrangian is a direct consequence of the scalar character of the action integral.[36,38,50] What this means is that both the functional probability density $\exp\left(-\int \mathscr{L}\, d\tau\right)$ and the measure in functional space are invariant under general coordinate transformations.[36,38,50],[7] Correspondingly, the Euler–Lagrange equations associated to (4.11) and (4.24) transform into each other,[8] and therefore, the latter define the most probable path corresponding to (4.1) in the primitive variables. We stress that, in accordance with the usual definition given at the beginning of Section 2, the most probable path is the path that satisfies the Euler–Lagrange equations corresponding to the extrema of the action integral. The concept of most probable path subject to various types of boundary conditions has been further analyzed in Refs. 51 and 52.

The Lagrangian (4.24) conserves the properties under time reversal that were discussed in Section 3: Its Euler–Lagrange equations are invariant under time reversal if the potential conditions (4.14) and (4.15) are assumed. These Euler–Lagrange equations are

$$
\begin{aligned}
&D_{\alpha\mu}^{-1}\left(\ddot{q}_\mu - \frac{\partial w_\mu}{\partial q_\nu}\dot{q}_\nu\right) \\
&\quad + (\dot{q}_\mu - w_\mu)\left[\frac{\partial D_{\alpha\mu}^{-1}}{\partial q_\nu}\dot{q}_\nu + D_{\nu\mu}^{-1}\frac{\partial w_\nu}{\partial q_\alpha} - \frac{1}{2}\frac{\partial D_{\nu\mu}^{-1}}{\partial q_\alpha}(\dot{q}_\nu - w_\nu)\right] \\
&\quad - \frac{\partial}{\partial q_\alpha}\left(\sqrt{D}\frac{\partial}{\partial q_\nu}\frac{w_\nu}{\sqrt{D}}\right) = 0
\end{aligned}
\tag{4.26}
$$

Equation (4.26) is invariant under time reversal if the following condition is fulfilled:

$$
\begin{aligned}
&\dot{q}_\mu\left[\frac{\partial}{\partial q_\alpha}(D_{\nu\mu}^{-1}w_\nu^I) - \frac{\partial}{\partial q_\mu}(D_{\alpha\nu}^{-1}w_\nu^I)\right] - D_{\nu\mu}^{-1}\left(\frac{\partial w_\nu^R}{\partial q_\alpha}w_\mu^I + \frac{\partial w_\nu^I}{\partial q_\alpha}w_\mu^R\right) \\
&\quad - \frac{1}{2}\frac{\partial D_{\nu\mu}^{-1}}{\partial q_\alpha}(w_\mu^R w_\nu^I + w_\mu^I w_\nu^R) - \frac{\partial}{\partial q_\alpha}\left(\sqrt{D}\frac{\partial}{\partial q_\nu}\frac{w_\nu^R}{\sqrt{D}}\right) = 0
\end{aligned}
\tag{4.27}
$$

[7] This remarkable property is not observed for ordinary probabilities, where in general the transformation law of the probability density involves a Jacobian. See, for example, (4.7).

[8] Note that if one directly applies the correspondence rule (2.33) to the Lagrangian (4.24) one does not obtain the correct Liouvillian (4.13). This is not surprising, since it reflects the fact that the correspondence rule to be used depends on the choice of coordinates if these are changed according to the usual rules of calculus.[53] The Lagrangian from which the Liouvillian (4.13) is obtained according to the symmetric ordering used in Section 2 is given in Ref. 24 and it differs from (4.24).

where, of course,

$$w_\mu{}^R = v_\mu{}^R \tag{4.28}$$

$$w_\mu{}^I = v_\mu{}^I - \sqrt{D}\,\frac{\partial}{\partial q_\nu}\frac{D_{\mu\nu}}{\sqrt{D}} \tag{4.29}$$

Although lengthy, it is a straightforward calculation to check that (4.14) and (4.15) imply the vanishing of the coefficient of $\dot{q}_\mu$ and of the remaining term in (4.27).

In the same way as it happened to the constant-diffusion Lagrangian, (4.24) is not invariant under time reversal, but there exists an invariant Lagrangian $\mathscr{L}^{\text{inv}}$ yielding the same Euler–Lagrange equations (4.26):

$$\mathscr{L}^{\text{inv}}(q,\dot{q}) = \frac{1}{4}\,D_{\mu\nu}^{-1}[(\dot{q}_\nu - w_\nu{}^R)(\dot{q}_\mu - w_\mu{}^R) + w_\mu{}^I w_\mu{}^I] + \frac{1}{2}\sqrt{D}\,\frac{\partial}{\partial q_\nu}\frac{w_\nu{}^I}{\sqrt{D}} \tag{4.30}$$

Assuming once again the potential conditions (4.14) and (4.15), we find that

$$\mathscr{L} - \mathscr{L}^{\text{inv}} = \frac{1}{2}\frac{d}{dt}(\phi_{\text{st}} - \log\sqrt{D}) \tag{4.31}$$

Comparing (4.31) with (4.21) and (3.13), we conclude the invariance under the change of variables (4.3) of $\mathscr{L} - \mathscr{L}^{\text{inv}}$, a quantity whose physical meaning was discussed earlier.

APPENDIX

An attempt to give a stochastic foundation to quantum mechanics was made some years ago by a number of authors.[29–31] We shall consider here only the work of de la Peña-Auerbach, which is representative of this line of research, and address ourselves to the question, "How can quantum mechanics, a time-reversal invariant theory, be reduced to a stochastic process which, as discussed in Section 3, exhibits irreversible behavior?". Writing the quantum mechanical wave function ψ in the form $\exp(R + iS)$, de la Peña-Auerbach has shown[30] that the probability density $P = \psi^*\psi$ can be taken to satisfy a FPE of the form

$$\partial P/\partial t = -\overline{\nabla}\cdot\bar{c}P + D_0\,\overline{\nabla}^2 P \tag{A1}$$

where $\bar{c}$ is the sum $\bar{v} + \bar{u}$ of a systematic velocity $\bar{v}$ and a stochastic component $\bar{u}$ that are given by

$$\bar{v} = 2D_0\,\overline{\nabla}S \tag{A2}$$

$$\bar{u} = 2D_0\,\overline{\nabla}R \tag{A3}$$

and $D_0 = \hbar/2m$. Under time reversal $\bar{v} \to -\bar{v}$ and $\bar{u} \to \bar{u}$,[30] so that $\bar{u}$ corresponds to what we have called v_μ^I, the irreversible drift, and $\bar{v}$ is the reversible drift v_μ^R. The derivation of a FPE for the quantum mechanical probability density is a crucial result of the so-called stochastic interpretation of quantum mechanics.[31]

Since quantum mechanics is a time-reversal invariant theory, consistency requires that the FPE (A1) be time-reversal invariant as well. This is indeed the case, and it is instructive to see how it comes about. From Eq. (A3) and the definition $P = e^{2R}$ of R we have

$$\bar{u} = D_0 \bar{\nabla} \log P \tag{A4}$$

or

$$-\bar{\nabla}\cdot(\bar{u}P) + D_0 \bar{\nabla}^2 P = 0 \tag{A5}$$

so that the two sources of irreversibility in the FPE, namely the irreversible drift and the diffusion, simply cancel one another at all times. Equation (A1) reduces to

$$\partial P/\partial t = -\bar{\nabla}\cdot\bar{v}P \tag{A6}$$

which is just the time-reversal invariant continuity equation for the quantum mechanical probability density. Although Eq. (A1) is formally similar to a FPE for a general diffusion process, nevertheless it fails to exhibit the key property of irreversibility that is normally associated with physical diffusion. In a sense the appearance of a FPE in this context is somewhat artifical: mathematically, it is seen to correspond to the simultaneous addition and subtraction of a diffusion term to Eq. (A6) through the use of (A4). It is also amusing to note that Eq. (A4) is of the same form as the potential condition (3.8) with the important difference that it is $\log P$ and not $\log P_{st}$ which appears in (A4). Clearly, such an extension of the potential condition from P_{st} to P goes far beyond detailed balance and implies a serious mutilation of the FPE. Indeed, Eq. (A4) means that the drift of (A1) is not an item external to that equation, but depends on the state of the system $P(q, t)$ at every time.

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