Quantum Langevin equation from forward–backward path integral

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Abstract

The quantum Langevin equation is derived from the Feynman–Vernon forward–backward path integral for a density matrix of a quantum system in a thermal oscillator bath. We exhibit the mechanism by which the classical, c-valued noise in the Feynman–Vernon theory turns into an operator-valued quantum noise. The quantum noise fulfills a characteristic commutation relation which ensures the unitarity of the time evolution in the quantum Langevin equation.

1. Introduction

The *quantum Langevin equation*

$$m\ddot{\hat{x}}_t + \gamma\dot{\hat{x}}_t + V'(\hat{x}_t) = \hat{\eta}_t \tag{1}$$

describes successfully the temporal behavior of a quantum mechanical point-like particle with the action

$$\mathcal{A}^S[x] = \int_0^t dt' [\tfrac{1}{2}m\dot{x}_t^2 - V(x_t)] \tag{2}$$

in the presence of dissipation [1,2]. The time argument is indicated by a subscript, for notational brevity. The dissipation is accounted for in Eq. (1) by the two phenomenological terms: the friction term $\gamma\dot{\hat{x}}_t$, and the quantum noise operator $\hat{\eta}_t$ which satisfies the commutation rules

$$[\hat{\eta}_t, \hat{\eta}_{t'}] = 2i\hbar\gamma\partial_t\delta(t - t') \tag{3}$$

and has the expectation values

$$\tfrac{1}{2}\langle[\hat{\eta}_t, \hat{\eta}_{t'}]_+\rangle_{\hat{\eta}} = K_T(t, t'), \tag{4}$$

with

$$K_T(t, t') = \frac{\gamma\hbar}{\pi} \int_0^\infty d\omega\,\omega\coth\frac{\hbar\omega}{2kT}\cos\omega(t - t'). \tag{5}$$

The prefactor γ is once more the friction constant, in accordance with the fluctuation–dissipation theorem. As usual, T denotes the temperature and k the Boltzmann constant. Remarkably, the temporal evolution governed by the quantum Langevin equation preserves the canonical commutation relation, i.e., quantizing $[\hat{x}_t, \hat{p}_t] = i\hbar$ with $\hat{p}_t = m\dot{\hat{x}}_t$ at one time, this remains true at all times [3].

The quantum Langevin equation (1) has been derived [4–6] from the Heisenberg equations of motion of the quantum system coupled to a thermal environment consisting of a bath of infinitely many harmonic oscillators. The coupling and the spectral distribution of the oscillators are chosen in such a way that the Heisenberg equations for the environment coordinates

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can be solved explicitly, and that the standard friction term arises in (1). The general procedure is described in Refs. [7,8].

The quantum Langevin equation can be used to derive *Kubo's stochastic Liouville equation* [9] for the temporal evolution of the density matrix of the system [3]. Solutions of this equation are in agreement with experimental data.

The same Kubo equation can be obtained [10] from a completely different description of the quantum system due to Feynman and Vernon [12,11]. Here the density matrix of the quantum system in an oscillator bath is represented by a path integral which contains a fluctuating noise variable η_t. In contrast to the quantum Langevin equation, the fluctuating noise in this formulation is classical.

In ordinary quantum mechanical path integrals, there exists a simple way of going from fluctuating classical variables to Heisenberg operators. For the classical fluctuating noise variable in the Feynman–Vernon path integral, on the other hand, the relation to the quantum noise operator $\hat{\eta}_t$ is unknown. The purpose of this paper is to exhibit this relation and to derive the quantum Langevin equation from the Feynman–Vernon path integral.

2. The forward–backward path integral for the density matrix of a system in a thermal bath

Consider the quantum mechanical system described by the action (2) in contact with an oscillator bath. The density operator $\hat{\rho}_t$ of the total system obeys the Neumann equation

$$i\hbar\partial_t\hat{\rho}_t = [\hat{H},\hat{\rho}_t], \tag{6}$$

where the Hamilton operator is the sum of three terms,

$$\hat{H} = \hat{H}^S + \hat{H}^B + \hat{H}^I. \tag{7}$$

The first term $\hat{H}^S$ describes the quantum system by itself, $\hat{H}^B$ the oscillators in the heat bath, and $\hat{H}^I$ the interaction of the system with the bath. A formal solution to Eq. (6) is

$$\hat{\rho}_t = \exp(-i\hat{H}t/\hbar)\,\hat{\rho}_0\exp(i\hat{H}t/\hbar). \tag{8}$$

Let X denote collectively an infinite set of oscillator coordinates in the heat bath. Then a matrix element of $\hat{\rho}_t$ has the time evolution

$$\langle xX|\hat{\rho}_t|x'X'\rangle = \int d\bar{x}\,d\bar{x}'\,d\bar{X}\,d\bar{X}'\,\langle xX|\,e^{-i\hat{H}t/\hbar}\,|\bar{x}\bar{X}\rangle$$
$$\times \langle \bar{x}\bar{X}|\hat{\rho}_0|\bar{x}'\bar{X}'\rangle\langle \bar{x}'\bar{X}'|\,e^{i\hat{H}t/\hbar}\,|x'X'\rangle. \tag{9}$$

By time-slicing the matrix elements of the two evolution operators on the right-hand side (one of them working forward, the other backward in time), they can be represented by corresponding path integrals [11–13],

$$\langle xX|\,e^{-i\hat{H}t/\hbar}\,|\bar{x}\bar{X}\rangle = \int \mathcal{D}x\,\mathcal{D}X\,e^{i\mathcal{A}[x,X]/\hbar}, \tag{10}$$

with the boundary conditions $x_0 = \bar{x}$, $x_t = x$ and $X_0 = \bar{X}$, $X_t = X$, and

$$\langle \bar{x}'\bar{X}'|\,e^{i\hat{H}t/\hbar}\,|x'X'\rangle = \int \mathcal{D}x'\,\mathcal{D}X'\,e^{-i\mathcal{A}[x',X']/\hbar}, \tag{11}$$

with the boundary conditions $x'_0 = \bar{x}'$, $x'_t = x'$ and $X'_0 = \bar{X}'$, $X'_t = X'$. The functional

$$\mathcal{A}[x,X] \equiv \mathcal{A}^S[x] + \mathcal{A}^B[X] + \mathcal{A}^I[x,X] \tag{12}$$

is the classical action associated with the Hamiltonian (7) of the total system.

We are interested in the temporal behavior of the system coordinate x_t regardless of the behavior of the environment variables X_t, i.e., we look for the so-called *reduced description* of the total quantum system. This is obtained by tracing out the environment coordinates in (9). The system and the bath may be assumed to be decoupled at some initial time, say $t = 0$. At that time, $\hat{\rho}_0 = \hat{\rho}_0^S\hat{\rho}_0^B$, and we can rewrite (9) as

$$\rho_t^S(x,x') \equiv \int dX\,\langle xX|\hat{\rho}_t|x'X\rangle$$
$$= \int dx_1\,dx'_1\,U_t(xx',x_1x'_1)\rho_0^S(x_1,x'_1), \tag{13}$$

where $U_t(xx',x_1x'_1)$ has the forward–backward path integral representation (the hyphen is pronounced *minus*)

$$U_t(xx', x_1 x_1') = \int \mathcal{D}x_+ \mathcal{D}x_-$$

$$\times F[x_+, x_-] \exp\frac{i}{\hbar}(\mathcal{A}^S[x_+] - \mathcal{A}^S[x_-]), \quad (14)$$

with $x_+(0) = x_1, x_+(t) = x, x_-(0) = x_1', x_-(t) = x'$. For variables with subscripts $\pm$ we place the time arguments in parentheses, to avoid a pile-up of subscripts. The functional

$$F[x_+, x_-] = \int d\bar{X} \, d\bar{X}' \rho_0^B(\bar{X}, \bar{X}')$$

$$\times \int dX \int \mathcal{D}X_+ \mathcal{D}X_- \exp\frac{i}{\hbar}(\mathcal{A}^I[x_+, X_+]$$

$$- \mathcal{A}^I[x_-, X_-] + \mathcal{A}^B[X_+] - \mathcal{A}^B[X_-]) \quad (15)$$

is Feynman's *influence functional* [11–13]. The forward–backward path integral over the bath coordinates is taken with the boundary conditions $X_+(0) = \bar{X}, X_+(t) = X, X_-(0) = \bar{X}'$ and $X_-(t) = X$.

The simplest bath action containing oscillators of frequency ω with coordinates $X_\omega(t)$ is

$$\mathcal{A}^B[X] = \frac{1}{2} \int_0^t dt' \int_0^\infty d\omega \, (\dot{X}_\omega^2 - \omega^2 X_\omega^2). \quad (16)$$

Assuming an initial equilibrium density operator for the bath,

$$\hat{\rho}_0^B = \exp(-\hat{H}^B/kT), \quad (17)$$

the interaction leading to the correct quantum Langevin equation is [3,13,14]

$$\mathcal{A}^I[x, X] = (2\gamma/\pi)^{1/2} \int_0^t dt' x \int_0^\infty d\omega \dot{X}_\omega. \quad (18)$$

Since all integrals are Gaussian, the influence functional can be calculated explicitly [11–13]. The result is

$$F[x_+, x_-] = F_0 \exp\left(\frac{i\gamma}{\hbar} \int_0^t dt' \, y\dot{x}\right)$$

$$\times \exp\left(-\frac{1}{2\hbar^2} \int_0^t dt' \, dt'' \, y_{t'} K_T(t', t'') y_{t''}\right) \quad (19)$$

$$\equiv \exp\left(\frac{i\gamma}{\hbar} \int_0^t dt' \, y\dot{x}\right) F_{fl}[y], \quad (20)$$

where we have introduced new variables

$$x \equiv \tfrac{1}{2}(x_+ + x_-), \quad y \equiv x_+ - x_-. \quad (21)$$

The constant $F_0 = F[0,0]$ in (19) is the initial value of the influence functional, where the system and bath are decoupled, i.e., $F_0 = \text{Tr}\,\hat{\rho}_0^B = \int dX \rho_0^B(X, X)$; the exponential in (20) is the dissipation part of the influence functional, while the functional $F_{fl}[y]$ describes thermal and quantum fluctuations. The two factors contribute in completely different ways to the Langevin equation.

Introducing a new function $\tilde{\rho}_t^S(x, y) \equiv \rho_t^S(x + \tfrac{1}{2}y, x - \tfrac{1}{2}y)$ and substituting (19) into (14) and (13), we obtain the evolution equation

$$\tilde{\rho}_t^S(x, y) = \int dx' \, dy' \, \tilde{U}_t^S(xy, x'y') \tilde{\rho}_0^S(x', y'), \quad (22)$$

where $\tilde{U}_t^S(xy, x'y')$ is given by the functional integral

$$\tilde{U}_t^S(xy, x'y') = F_0 \int \mathcal{D}x \mathcal{D}y \, \exp(i\mathcal{A}_T[x, y]/\hbar), \quad (23)$$

with the boundary conditions $x_0 = x', x_t = x, y_0 = y', y_t = y$. The temperature-dependent action is

$$\mathcal{A}_T[x, y] = \int_0^t dt' \left(m\dot{y}\dot{x} - \gamma y\dot{x}\right.$$

$$\left. - V(x + \tfrac{1}{2}y) + V(x - \tfrac{1}{2}y) + \frac{i}{2\hbar} y\hat{K}_T y\right). \quad (24)$$

For brevity, we have written $\hat{K}_T y_{t'}$ for the integral $\int_0^t dt'' \, K_T(t', t'') y_{t''}$ in the last term. Due to this term, the temperature-dependent action is nonlocal in time. Note that at $t = 0$, $U_0^S(xy, x'y')$ reduces to $F_0\delta(x - x')\delta(y - y')$.

The temporal nonlocality of the action (24) can be removed by means of a random *noise* variable with the correlation function

$$\langle \eta_t \eta_{t'} \rangle_\eta = K_T(t, t'). \quad (25)$$

We simply make use of the Gaussian identity

$$\exp\left(-\frac{1}{2\hbar^2}\int\limits_0^t dt'\, y\hat{K}_T y\right)$$

$$= \int \mathcal{D}\eta \exp \int\limits_0^t dt' \left(-\frac{1}{2}\eta\hat{K}_T^{-1}\eta + \frac{i}{\hbar}\eta y\right)$$

$$\equiv \left\langle \exp\left(\frac{i}{\hbar}\int\limits_0^t dt' y\eta\right)\right\rangle_\eta \qquad (26)$$

associated with (25). Thus, if we agree to average all equations at the end with respect to the noise variable, we may replace the effective action in the evolution operator (23) by

$$\mathcal{A}_\eta[x, y] = \int\limits_0^t dt'\, [m\dot{y}\dot{x} - \gamma y\dot{x}$$

$$- V(x + \tfrac{1}{2}y) + V(x - \tfrac{1}{2}y) + y\eta]. \qquad (27)$$

In the limit of high temperatures, the noise fluctuations become large and local,

$$\langle\eta_t\eta_{t'}\rangle_\eta = K_T(t, t') = 2kT\gamma\delta(t - t') + O(1/T). \qquad (28)$$

Eq. (26) shows that the average size of the fluctuating variable y goes to zero like $\hbar/\sqrt{kT}$. Hence the action (24) becomes local, the potential difference $V(x + \tfrac{1}{2}y) - V(x - \tfrac{1}{2}y)$ can be approximated by $V'(x)y$, and (27) turns into

$$\mathcal{A}_\eta[x, y] = \int\limits_0^t dt'\, [-m\ddot{x} - \gamma\dot{x} - V'(x) + \eta]y. \qquad (29)$$

An integration by parts has been performed in the first term of the integrand in (27), absorbing a boundary term in the prefactor of the path integral (23). We can now perform the functional integral over y and find the classical version of the Langevin equation (1),

$$m\ddot{x}_t + \gamma\dot{x}_t + V'(x_t) = \eta_t, \qquad (30)$$

which describes classical Brownian motion. The classical behavior at large T is a consequence of $\hbar$ and T appearing in the combination $\hbar\omega/2kT$ in (5), so that $T \to \infty$ is equivalent to $\hbar \to 0$.

There have been attempts to include quantum effects into this classical equation by simply replacing the local noise correlation (28) by the finite temperature one (25), while maintaining the linear approximation $V'(x)y$ to $V(x + \tfrac{1}{2}y) - V(x - \tfrac{1}{2}y)$. The result has been called a *quasiclassical Langevin equation* [14,15]. Obviously, such an approximation can be reasonable only for nearly harmonic potentials (see also the remarks in Ref. [10], p. 589).

It is surprising that by converting the variables x_t and η_t in (30) into operators in (1), *all* terms in the expansion of $V(x + \tfrac{1}{2}y) - V(x - \tfrac{1}{2}y)$ in powers of y can be accounted for, as we shall prove.

3. Kubo's stochastic Liouville equation

Eqs. (22) and (23) resemble the evolution equation of a Schrödinger wave function whose role is now played by the density function $\tilde{\rho}_t^S(x, y)$. This analogy is helpful in deriving a Schrödinger-like differential equation for $\tilde{\rho}_t^S$. This equation is most easily found by going over from a Lagrange-type path integral (23) to a Hamiltonian one, expressed in terms of the position and canonical momentum variables (see Section 18.6 in Ref. [13]). The effective action (24) goes over into

$$\mathcal{A}_T[x, y] \to \mathcal{A}_T[p_x, p_y, x, y]$$

$$= \int\limits_0^t dt'\, (p_x\dot{x} + p_y\dot{y} - H_T), \qquad (31)$$

where

$$H_T = \frac{1}{m}(p_x + \gamma y)p_y$$

$$+ V(x + \tfrac{1}{2}y) - V(x - \tfrac{1}{2}y) - \frac{i}{2\hbar}y\hat{K}_T y \qquad (32)$$

plays the role of a Hamiltonian. For the noise-dependent effective action (27) we find an analogous action $\mathcal{A}_\eta[p_x, p_y, x, y]$ involving the Hamiltonian

$$H_\eta = \frac{1}{m}(p_x + \gamma y)p_y + V(x + \tfrac{1}{2}y) - V(x - \tfrac{1}{2}y) - y\eta. \qquad (33)$$

Using the effective action (31), we obtain the alternative path integral representation for the time evolution operator in (22),

$$\tilde{U}_t^S(xy, x'y')$$

$$= \tilde{F}_0 \int \mathcal{D}p_x \, \mathcal{D}p_y \, \mathcal{D}x \, \mathcal{D}y \, \exp \mathrm{i} \mathcal{A}_T[p_x, p_y, x, y]/\hbar. \tag{34}$$

A similar equation holds for a fixed noise with the action $\mathcal{A}_\eta[p_x, p_y, x, y]$.

Since the action $\mathcal{A}_\eta[p_x, p_y, x, y]$ is local in time, we conclude that for a fixed noise η, the associated noise-dependent (*noisy*) density matrix $\tilde{\rho}_t^S[\eta]$ obeys the Schrödinger-like equation

$$\mathrm{i}\hbar \dot{\tilde{\rho}}_t^S[\eta] = \hat{H}_\eta \tilde{\rho}_t^S[\eta], \tag{35}$$

with $\hat{H}_\eta$ being the operator arising from (33) by substituting $p_x \rightarrow -\mathrm{i}\hbar\partial_x, p_y \rightarrow -\mathrm{i}\hbar\partial_y$. The noise average of the solution to (35) is the density matrix of the system,

$$\tilde{\rho}_t^S(x, y) = \langle \tilde{\rho}_t^S[\eta] \rangle_\eta. \tag{36}$$

Eq. (35) supplemented by (25) and (36) is called Kubo's stochastic Liouville equation [9], which we have thus derived from the Feynman–Vernon forward-backward path integral.

Note that there is no analogous procedure to obtain a differential equation for the density matrix $\tilde{\rho}_t^S(x, y)$ from the Hamiltonian (32), due to the nonlocality of the $\hat{K}_T$ term. Only in the limit of large temperatures, when H_T becomes local due to (28), there exists a Schrödinger-like equation which is the Fokker–Planck equation at finite friction.

It must be pointed out that the transition from the Hamiltonians H_T and H_η to their operators has an ordering ambiguity in the term $\gamma y p_y/m$ in $\hat{H}_T$ and $\hat{H}_\eta$ (see Section 18.6 in Ref. [13]). In the time-sliced path integral we must decide whether to write $\gamma y_n p_{y\,n}/m$ or $\gamma y_n p_{y\,n-1}/m$ where the subscript n numbers the time slice. Since the ordering is independent of temperature, we resolve the ambiguity in the limit of large temperatures: from the well-known Fokker–Planck equation we determine the correct operator ordering of the term $\gamma y p_y/m$ to be $-\mathrm{i}\hbar\gamma y \partial_y/m$.

4. Classical noise versus quantum noise

The noise in Kubo's equation is a c-number, and its relation to an operator-valued noise of the quantum

Langevin equation (1) has been an outstanding puzzle, as pointed out in Section 1. To find this relation, we observe that it is possible to remove the temporal nonlocality in the initial effective action (24) just as easily with the help of an operator-valued noise $\hat{\eta}$. This was, in fact, how the Feynman–Vernon path integral was derived in Ref. [13] (see Eq. (18.162)). An operator-valued noise possessing the properties (3), (4) can be chosen as a sum of all Heisenberg operators of the oscillator velocities. Explicitly

$$\hat{\eta}_t = \sqrt{2\gamma/\pi} \, \partial_t \int_0^\infty \mathrm{d}\omega \, \mathrm{e}^{\mathrm{i}\hat{H}^\mathrm{B}t/\hbar} \, \hat{X}_\omega \, \mathrm{e}^{-\mathrm{i}\hat{H}^\mathrm{B}t/\hbar} \tag{37}$$

$$= \mathrm{i}(\gamma/\pi)^{1/2} \int_0^\infty \mathrm{d}\omega \, \sqrt{\omega}(\mathrm{e}^{\mathrm{i}\omega t} \hat{a}_\omega^\dagger - \mathrm{e}^{-\mathrm{i}\omega t} \hat{a}_\omega), \tag{38}$$

where $\hat{a}_\omega^\dagger$ and $\hat{a}_\omega$ are time-independent creation and annihilation operators with the usual commutation rules,

$$[\hat{a}_\omega, \hat{a}_{\omega'}] = 0, \quad [\hat{a}_\omega^\dagger, \hat{a}_{\omega'}^\dagger] = 0,$$
$$[\hat{a}_\omega, \hat{a}_{\omega'}^\dagger] = \hbar\delta(\omega - \omega'). \tag{39}$$

The noise operator (38) satisfies the commutation rule (3). The correlation function (4) follows if we define $\hat{\eta}$-averages as bath averages,

$$\langle [\hat{\eta}_t, \hat{\eta}_{t'}]_+ \rangle_{\hat{\eta}} \equiv \mathrm{Tr}\,(\hat{\rho}_0^\mathrm{B} [\hat{\eta}_t, \hat{\eta}_{t'}]_+). \tag{40}$$

Thus the operator (37) has precisely the properties of the quantum noise variable in the quantum Langevin equation (1).

In the operator representation of the noise variable, the influence functional is given by (see Eq. (18.162) in Ref. [13])

$$F[x_-, x_+] = \mathrm{Tr}\left[\hat{\rho}_0^\mathrm{B} \hat{T}_\mathrm{C} \exp\left(\frac{\mathrm{i}}{\hbar} \int_\mathrm{C} \mathrm{d}t' x_\mathrm{C} \hat{\eta}_\mathrm{C}\right)\right], \tag{41}$$

where C is a closed-time contour encircling tightly the interval $[0, t]$ in the complex t plane and $\hat{T}_\mathrm{C}$ is the ordering operator along this contour. The subscript C distinguishes the upper and lower branches of the integration contour, where $x_\mathrm{C}(t)$ is equal to $x_+(t)$ and $x_-(t)$, respectively, whereas the operator $\hat{\eta}_\mathrm{C}$ is equal

to $\hat{\eta}_t$ on both branches. Introducing the symbol $\hat{T}^{-1}$ to denote anti-time ordering, Eq. (41) takes the more explicit form

$$F[x_-, x_+] = \text{Tr} \left[\hat{\rho}_0^B \hat{T}^{-1} \exp\left(-\frac{i}{\hbar} \int_0^t dt' \, x_- \hat{\eta} \right) \right.$$

$$\left. \times \hat{T} \exp\left(\frac{i}{\hbar} \int_0^t dt' \, x_+ \hat{\eta} \right) \right]. \tag{42}$$

Assuming the explicit noise representation (37) through the heat bath operators we observe that the matrix element $\langle \bar{X} | \hat{T} \exp(i \int_0^t dt' \, x_+ \hat{\eta}/\hbar) | X \rangle$ and the corresponding matrix element of the anti-time ordered exponential in (42) are given by the path integrals over X_+ and X_- in (15), respectively, whereas the trace in (42) corresponds to the integrals over $X, \bar{X}$ and $\bar{X}'$ in (15).

We now make the key observation that will allow us to derive the quantum Langevin equation (1): The fluctuation part of the influence functional, defined in Eq. (20), is obtained from (42) by setting $x = 0$. Then both exponentials in (42) carry the same argument $(i/2\hbar) \int_0^t dt' \, y \hat{\eta}$. When expanding the product of the two exponentials in a power series and performing the proper time orderings, the bath average can be rewritten as

$$F_{\text{fl}}[y] = F[\tfrac{1}{2}y, -\tfrac{1}{2}y]$$

$$= \text{Tr} \left[\hat{T} \exp\left(\frac{i}{\hbar} \int_0^t dt' \, y_t \, \text{ad} \, \hat{\eta}_t \right) \hat{\rho}_0^B \right], \tag{43}$$

where ad $\hat{\eta}_t$ is the adjoining operator associated with the noise operator $\hat{\eta}_t$. This is defined as follows. When acting upon an arbitrary operator $\hat{O}$, the adjoining operator is equal to half the anticommutator,

$$\text{ad} \, \hat{\eta}_t \, \hat{O} \equiv \tfrac{1}{2} [\hat{\eta}_t, \hat{O}]_+. \tag{44}$$

The bath average (43) corresponds to defining a noise average of an arbitrary functional $\mathcal{O}[\text{ad} \, \hat{\eta}]$ by

$$\langle \mathcal{O}[\text{ad} \, \hat{\eta}] \rangle_{\hat{\eta}}^{\text{ad}} \equiv \text{Tr} \, \mathcal{O}[\text{ad} \, \hat{\eta}] \hat{\rho}_0^B. \tag{45}$$

Note that the adjoining operator ad $\hat{\eta}$ acts also upon $\hat{\rho}_0^B$. The ket superscript ad emphasizes this fact which is in contrast to averages with respect to the ordinary

noise operator defined as in (40). For example, the correlation function is calculated as

$$\langle \text{ad} \, \hat{\eta}_t \, \text{ad} \, \hat{\eta}_{t'} \rangle_{\hat{\eta}}^{\text{ad}} = \tfrac{1}{4} \text{Tr} \, [\hat{\eta}_t, [\hat{\eta}_{t'}, \hat{\rho}_0^B]_+]_+$$

$$= \tfrac{1}{2} \text{Tr} \, \hat{\rho}_0^B [\hat{\eta}_t, \hat{\eta}_{t'}]_+ = K_T(t, t'). \tag{46}$$

The adjoining operator ad $\hat{\eta}_t$ has an important property crucial to the further development: Although the original noise operator $\hat{\eta}_t$ has a nontrivial commutator (3) with itself at a different time, two adjoining operators ad $\hat{\eta}_t$ and ad $\hat{\eta}_{t'}$ commute with each other, so that they can be treated as c-numbers. Indeed, for an arbitrary operator $\hat{O}$ we verify that

$$[\text{ad} \, \hat{\eta}_t, \text{ad} \, \hat{\eta}_{t'}] \hat{O} = [\hat{\eta}_t, \hat{\eta}_{t'}] \hat{O} + \hat{O} [\hat{\eta}_{t'}, \hat{\eta}_t] = 0. \tag{47}$$

In all such calculations, we may treat the quantum noise ad $\hat{\eta}_t$ as if it were a classical noise η_t.

Furthermore, it is clear from the action (16) that ad $\hat{\eta}_t$ is a Gaussian noise variable, just as the classical η_t. The correlation functions of any number of operators ad $\hat{\eta}_t$ evaluated in the average (45) are completely specified by their two-point function (46) following Wick's expansion rule. Since the expectation values of the products of two η_t or of two ad $\hat{\eta}_t$ are identical, $\langle \eta_t \eta_{t'} \rangle_\eta \equiv \langle \text{ad} \, \hat{\eta}_t \, \text{ad} \, \hat{\eta}_{t'} \rangle_{\hat{\eta}}$, all correlation functions must be identical as well – quantum and classical noises are completely equivalent.

Substituting (43) into (23) and repeating the arguments leading to Kubo's equation in Section 3, we again end up with a modification of Kubo's stochastic Liouville equation, in which the noise is operator-valued, i.e., η_t in (35) and (36) is replaced by ad $\hat{\eta}_t$.

Having shown how the operator-valued quantum noise turns into a classical noise in Kubo's stochastic Liouville, we are ready to derive the quantum Langevin equation (1).

5. Quantum Langevin equation

As the first step, we derive the evolution equation for the system's density matrix operator $\hat{\rho}_t^S$ whose matrix elements are defined by (13). Its operator representation is $\hat{\rho}_t^S = \text{Tr}_B \, \hat{\rho}_t$ where Tr_B denotes the trace over bath degrees of freedom. Returning in Kubo's equation (35) to the initial forward–backward vari-

ables $x_\pm$ of (21), we find the evolution equation for the noisy matrix elements associated with (13),

$$i\hbar\partial_t\rho_t^S(x_+, x_-)$$
$$= [\hat{H}_+^S - \hat{H}_-^S + (\gamma/2m)(\hat{x}_+ - \hat{x}_-)(\hat{p}_+ - \hat{p}_-)$$
$$- (\hat{x}_+ - \hat{x}_-)\,\text{ad}\,\hat{\eta}_t]\rho_t^S(x_+, x_-), \qquad (48)$$

where $\hat{p}_\pm \equiv -i\hbar\partial/\partial x_\pm$, and $\hat{H}_\pm^S = H^S(\hat{p}_\pm, \hat{x}_\pm)$ is the system Hamiltonian expressed in terms of the forward–backward phase space variables.

Of course, this equation can also be obtained directly from Eq. (9). The Hamilton operators in the two exponentials yield directly the difference $\hat{H}_+^S - \hat{H}_-^S$ in (48), whereas the other two terms result from the dissipation and fluctuation parts of the influence functional in the path integral (14).

Let $|x\rangle$ and $|p\rangle$ denote eigenvectors of the canonically conjugate system operators $\hat{x}$ and $\hat{p}$, respectively. Then $\rho_t^S(x_+, x_-) = \langle x_+|\hat{\rho}_t^S|x_-\rangle$. We have the following identities:

$$(\hat{H}_+^S - \hat{H}_-^S)\langle x_+|\hat{\rho}_t^S|x_-\rangle = \langle x_+|[\hat{H}^S, \hat{\rho}_t^S]|x_-\rangle, \quad (49)$$

$$(\hat{x}_+\hat{p}_+ + \hat{x}_-\hat{p}_-)\langle x_+|\hat{\rho}_t^S|x_-\rangle$$
$$= \langle x_+|(\hat{x}\hat{p}\hat{\rho}_t^S - \hat{\rho}_t^S\hat{p}\hat{x})|x_-\rangle, \qquad (50)$$

$$(\hat{x}_-\hat{p}_+ + \hat{x}_+\hat{p}_-)\langle x_+|\hat{\rho}_t^S|x_-\rangle$$
$$= \langle x_+|(\hat{p}\hat{\rho}_t^S\hat{x} - \hat{x}\hat{\rho}_t^S\hat{p})|x_-\rangle, \qquad (51)$$

which can be proved by inserting suitable resolutions of unity, $\int dp|p\rangle\langle p| = \int dx|x\rangle\langle x| = 1$, between the operators on the right-hand sides. Substituting Eqs. (49)–(51) into (48), we find the evolution equation for the operator $\hat{\rho}_t^S[\text{ad}\,\hat{\eta}]$,

$$i\hbar\partial_t\hat{\rho}_t^S = [\hat{H}^S, \hat{\rho}_t^S] + \tfrac{1}{2}[\hat{x}, [\gamma\hat{p}/m - \hat{\eta}_t, \hat{\rho}_t^S]_+]. \quad (52)$$

The average (45) of a solution to (52) gives the density matrix operator of the system

$$\hat{\rho}_t^S = \langle\hat{\rho}_t^S[\text{ad}\,\hat{\eta}]\rangle_{\hat{\eta}} = \text{Tr}_B\,\hat{\rho}_t^S[\text{ad}\,\hat{\eta}]\rho_0^B. \qquad (53)$$

Now we turn directly to a derivation of equations of motion for system operators. Let us recall first that in quantum mechanics there are two equivalent representations of the mean value $\langle\hat{O}\rangle_t$ of any dynamical variable $\hat{O}$ (with or without explicit time dependence) at a time t

$$\langle\hat{O}\rangle_t = \text{Tr}\,\hat{O}\hat{\rho}_t = \text{Tr}\,\hat{O}_t\hat{\rho}_0, \qquad (54)$$

where $\hat{\rho}_t^S$ is the density matrix operator at the time t, and $\hat{O}_t$ is the Heisenberg operator coinciding with $\hat{O}$ at $t = 0$. The first equality expresses the mean-value in the Schrödinger picture, while the second one determines it in the Heisenberg representation. Eq. (54) can also be regarded as a definition of the Heisenberg operator $\hat{O}_t$. The consistency of this definition is guaranteed by the time independence of the commutation relations $[\hat{O}, \hat{O}'] = [\hat{O}_t, \hat{O}_t']$ for any two operators. This, in turn, is a consequence of the unitarity of the temporal evolution of the density matrix described by the Neumann equation (6).

The evolution of a quantum systems with dissipation is determined by a generalization of the Neumann equation (52). We shall demonstrate in analogy with (54), that there exists a consistent definition of noisy Heisenberg operators, if the noise obeys the commutation relation (3). For any product of system operators $\hat{O}^S = \prod_{k=1}^n \hat{O}^{(k)}$, a product of noisy Heisenberg system operators is defined by the equality

$$\text{Tr}_S\,\hat{O}^S\hat{\rho}_t^S[\text{ad}\,\hat{\eta}] = \text{Tr}_S\prod_{k=1}^n \hat{O}^{(k)}\hat{\rho}_t^S[\text{ad}\,\hat{\eta}]$$

$$\equiv \text{Tr}_S\prod_{k=1}^n \hat{O}_t^{(k)}[\hat{\eta}]\hat{\rho}_0^S = \text{Tr}_S\,\hat{O}_t^S[\hat{\eta}]\hat{\rho}_0^S, \qquad (55)$$

where the noisy density matrix operator satisfies Kubo's stochastic Eq. (52), and Tr_S implies a trace over system degrees of freedom. One can think of relation (55) as a mapping of an algebra of system operators at the time $t = 0$ onto their algebra at a time t. Taking a trace of the evolution equation (52), we see that the unit operator $\hat{I}$ remains invariant under the mapping (55), i.e., $\dot{\hat{I}}_t[\hat{\eta}] = 0$, so that $\hat{I}_t[\hat{\eta}] \equiv \hat{I}$. The consistency of the definition (55) is guaranteed by the time independence of the commutation relations

$$[\hat{O}^S, \hat{O}'^S] = [\hat{O}_t^S[\hat{\eta}], \hat{O}_t'^S[\hat{\eta}]], \qquad (56)$$

for any two $\hat{O}_t^S[\hat{\eta}]$ and $\hat{O}_t'^S[\hat{\eta}]$. At $t = 0$, Eq. (56) is trivially fulfilled. To prove the time independence, we derive the noisy Heisenberg equation for $\hat{O}_t^S$. Differentiating (55) with respect to time and making use of both (52) and (55), we obtain

$$i\hbar\dot{\hat{O}}_t^S = [\hat{O}_t^S, \hat{H}_t^S] + \tfrac{1}{2}(\gamma\hat{p}_t/m - \hat{\eta}_t, [\hat{O}_t^S, \hat{x}_t])_+, \qquad (57)$$

where $\hat{H}_t^S = H^S(\hat{p}_t, \hat{x}_t)$. For a noise operator satisfying the commutation rule (3), this equation leads indeed to (56) (see Ref. [3]). Equivalently, we demonstrate that Eq. (57) coincides with the Heisenberg equations of motion of the entire system (the particle in a heat bath), comprising the quantum Langevin equation (1).

For an arbitrary system operator we have

$$i\hbar\dot{\hat{O}}_t^S = [\hat{O}_t^S, \hat{H}_t] = [\hat{O}_t^S, \hat{H}_t^S]$$
$$+ \frac{1}{2}\left(\frac{2\gamma}{\pi}\right)^{1/2}\left(\int_0^\infty d\omega \, \hat{X}_{\omega t}, [\hat{O}_t^S, \hat{x}_t]\right)_+, \quad (58)$$

$$i\hbar\dot{\hat{X}}_{\omega t} = [\hat{X}_{\omega t}, \hat{H}_t], \quad i\hbar\dot{\hat{P}}_{\omega t} = [\hat{P}_{\omega t}, \hat{H}_t], \quad (59)$$

where $\hat{H}_t$ is the canonical Hamilton operator corresponding to the total action (12) defined by (2), (16) and (18),

$$\hat{H}_t = \hat{H}_t^S + \hat{H}_t^B + \hat{H}_t^I = \hat{H}_t^S$$
$$+ \frac{1}{2}\int_0^\infty d\omega\{[\hat{P}_{\omega t} - (2\gamma/\pi)^{1/2}\hat{x}_t]^2 + \omega^2\hat{X}_{\omega t}^2\}.$$
$$(60)$$

The ω-integral in this Hamiltonian produces a linearly divergent term $\propto \frac{1}{2}\hat{x}^2$, the "frequency shift term" discussed at length in Ref. [10]. The divergence is due to the specific form of the interaction (18) which generates the desired time-independent friction coefficient γ in the Langevin equation [7]. The same divergence appears also in the Hamiltonian form of the forward–backward path integral (14). The divergence is canceled by an equal divergence in the dissipation part of the influence functional arising from the coupling to momenta of heat bath oscillators (the term $\sim xP_\omega$ in (60)) [10, p. 602]. For this reason, Kubo's stochastic equation has only finite terms. This pleasant cancellation is absent if the system is coupled directly to the positions of the bath oscillators rather than to their velocities, as in (18). In that case, the initial potential $V(x)$ requires a divergent counter term in order to obtain a finite Kubo equation. The entire issue is, of course, somewhat academic since it is a consequence of insisting upon a constant friction, which is physical only at low frequencies, much lower than the collision rate in the system. For larger frequencies, the

physical behavior is described by the Drude friction $\gamma(\omega) \propto 1/(1 + \omega^2/\omega_D^2)$, and there is no divergence at all [7] (see also Eq. (3.156) in Ref. [13]).

Imagining the presence of a frequency cutoff in (60), we solve the oscillator Heisenberg equations (59) and find

$$\left(\frac{2\gamma}{\pi}\right)^{1/2}\int_0^\infty d\omega \, \hat{X}_{\omega t} = \gamma\dot{\hat{x}}_t - \hat{\eta}_t = \gamma\hat{p}_t/m - \hat{\eta}_t, \quad (61)$$

where we have used the representation (38) for the noise operator. Substituting (61) into (58) and comparing it with (57) we conclude that

$$\hat{O}_t^S[\hat{\eta}] = e^{i\hat{H}t/\hbar}\,\hat{O}^S\,e^{-i\hat{H}t/\hbar} = \hat{O}_t^S. \quad (62)$$

Thus, the solutions of the evolution equation (57) coincide with Heisenberg system operators. Hence, the temporal evolution is unitary and (56) holds. Note that the system Hamiltonian is no longer an integral of motion, $d\hat{H}_t^S/dt \neq 0$, in contrast with the Hamiltonian driving the ordinary Heisenberg equations.

Setting $\hat{O}_t^S$ equal to $\hat{x}_t$ and $\hat{p}_t$ in Eq. (57) or, equivalently, in Eq. (58), we obtain the Heisenberg equations of motion,

$$\dot{\hat{x}}_t = \hat{p}_t/m, \quad (63)$$

$$\dot{\hat{p}}_t = -V'(\hat{x}_t) - \gamma\hat{p}_t/m + \hat{\eta}_t, \quad (64)$$

which are equivalent to (1)

Eq. (62) ensures the unitarity of the temporal evolution and the time independence of the canonical commutation relation $[\hat{x}_t, \hat{p}_t] = i\hbar$. This guarantees also that correlation functions of noisy operators within the $\hat{\eta}$ average agree with the ordinary quantum-mechanical correlation functions of the system described by the Hamilton operator (60),

$$\mathrm{Tr}_S\,\hat{\rho}_0^S\langle[\hat{O}_t^S[\hat{\eta}], \hat{O}_{t'}'^S[\hat{\eta}]]\rangle_{\hat{\eta}} = \mathrm{Tr}\,\hat{\rho}_0[\hat{O}_t^S, \hat{O}_{t'}'^S].$$
$$(65)$$

The property (3) of the quantum noise is crucial for the unitarity of the time evolution of the Heisenberg operators. To see what happens if the noise were commutative, we replace ad $\hat{\eta}$ in (52) by a c-valued Gaussian noise η, which we are apparently allowed to do after the above observations on the equivalence of averages. Then we can again define the noisy Heisenberg representation by (55) and derive (57) in a simi-

lar way. However, we can never prove the consistency of (57) and (55); Eqs. (56) and (62) are no longer valid. For a commutative noise, the violation of the canonical commutation relation as time proceeds is seen from (63), (64), most simply for $V = 0$. This breakdown of the unitarity in the temporal evolution would prevent us from identifying (57) with the quantum Langevin equation.

Thus we have shown that the Feynman–Vernon path integral description of quantum Brownian motion is completely equivalent to a description in terms of the quantum Langevin equation (1). Both descriptions can be used on equal footing to study dissipative processes in quantum mechanics.

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