Path-integral formalism for classical Brownian motion in a general environment

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The path-integral formalism for classical Brownian motion in a general environment is derived from the first principles of microdynamics by using the path-integral formulation of classical mechanics. The classical influence functional, which contains a nonlocal dissipation term and a colored noise term, is introduced. We show that there exists a classical fluctuation-dissipation relation. We also compare this classical influence functional theory with the well-known quantum influence-functional theory.

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The trajectory of a classical particle in phase space is uniquely determined by Newton's equations (or Hamilton's equations) with given initial conditions. However, if the particle is influenced by external stochastic forces (usually called noise), its classical trajectory is no longer uniquely determined. It can travel through phase space by many different paths, and a statistical probability can be assigned to each physically allowed trajectory. Taking the average over these different paths is equivalent to taking a path integral. In principle, there exists a path-integral formulation for classical Brownian motion.

The path-integral formulation for classical free diffusive Brownian motion under the influence of white noise is well known.

$$J(x_f,t|x_i,0)=N\int_{x_i}^{x_f}Dx\,\exp\left\{-\frac{\gamma_0}{2kT}\int_0^t ds\,\tfrac{1}{2}\dot{x}^2\right\}. \quad (1)$$

It is the Wiener integral in statistical physics [1], where $J(x_f,t|x_i,0)$ is the phase-space conditional probability, γ_0 is the damping constant (assumed very large since it is diffusive motion), T is the temperature, and the external potential $V(x)$ is zero.

In a general environment, the Brownian motion can be very complicated. The noise can be colored and the damping force can contain a memory function, so the Brownian motion can be non-Markovian [2]. The non-Markovian character strongly influences the dynamics, such as Kramers rate in bistable systems [3] or angular-momentum autocorrelation functions of rotational Brownian motion in some molecular systems [4]. The path-integral formalism may help us to understand the classical Brownian motion in a more general environment.

To set up a path-integral formulation for a classical Brownian particle in *a general environment* is a difficult problem and has been found only in some limiting cases. Among these previous works, Dykman and co-workers [5] first reported the path-integral formulation for a Brownian particle with white noise and a linear local damping force (the damping constant is not necessarily very large); Stratonovich [6], and more recently, McKane, Luckock, and Bray [7] formulated the path-integral formulation for a diffusive Brownian particle with colored noise and a local damping force (no memory function). All these previous works were derived from a phenomenological (generalized) Langevin equation instead of the first principles of microdynamics.

In quantum stochastic dynamics, a path-integral formulation of the quantum Brownian motion in a general environment was developed long ago. Feynman and Vernon first introduced the *quantum influence-functional theory* [8]. Since then, this quantum path-integral formulation has been generalized to more complicated cases, even to quantum stochastic fields [9]. The quantum master equations also have been derived by using this path-integral formalism [10].

This paper reports a path-integral formulation for *classical* Brownian motion with a general nonlocal dissipation and colored noise derived from the first principles of classical microdynamics. We have developed a *classical influence-functional theory* to treat the nonlocal dissipation and the colored noise. This classical theory could be viewed as a classical analogy of the quantum influence-functional theory. The reason why the quantum theory had been developed long before the classical theory in this particular problem is that, unlike quantum mechanics, the *path-integral formulation for classical mechanics* [11] has been only very recently discovered.

We consider a Brownian particle (the system) interacting with its environment (the bath), which is assumed to be very large and at thermal equilibrium. We use a set of harmonic oscillators to model the environment. The system plus environment is defined to be a closed system so we can use Newtonian mechanics to describe its motion. The dynamics of the Brownian particle can be obtained by averaging away the dynamics of the bath variables over some statistical ensemble of the initial conditions of

the bath variables.

The standard method to reduce the dynamics of the system plus environment to the dynamics of the system (the Brownian particle in our case) is the *projection operator method* [12]. Zwanzig used this system-bath model to derive a Langevin equation and to illustrate the concepts of noise and damping [13]. However, the projection operator method usually first gives a master equation (such as a Fokker-Planck equation) or a stochastic dynamics equation (such as Langevin equation). Additional work is required to convert the master equation or the stochastic dynamics equation to the path-integral formulation. In this letter, as another purpose of this work, we develop a new method to carry out the reduction of the dynamics of the system plus environment to the dynamics of the system and derive a path-integral formulation for the classical Brownian motion from microdynamics.

The new method is based on the *path-integral formulation of classical mechanics* [11] developed very recently in a study of hidden supersymmetries in classical mechanics. It appears quite meaningless to apply path integrals to *pure* classical mechanics (not containing any stochastic forces) because there is only one physical path with any given initial conditions (so the probability for this physical path is one and is zero for other possible paths). However, this *path-integral of classical mechanics* allows us to carry out the average over dynamics of the bath variables in a very simple and explicit way. A *classical influence functional* in the classical path integral is introduced. All the influence of the bath variables is now contained in this functional. After this averaging procedure, since it is already in path-integral form, we automatically obtain the path-integral formulation for classical Brownian motion.

Let us consider a Brownian particle with mass M and external potential $V(x)$. Its environment is a set of harmonic oscillators with mass m_n and natural frequency ω_n. The particle is coupled linearly to each bath oscillator with strength C_n. The Hamiltonian of the combined system plus environment is

$$H[x,p,q,k]=\{(p^2/2M)+V(x)\}+\sum_n\{(k_n^2/2m_n)+\tfrac{1}{2}m_n\omega_n^2q_n^2\}+\sum_n\{C_nxq_n\}\ , \quad (2)$$

where x and p, q_n and k_n are the coordinate and canonical momentum of the Brownian particle and the nth bath oscillator, respectively. The classical Hamilton's equations are

$$\dot{\phi}^a(t)=\omega^{ab}\partial_b H[\phi(t)]\ , \quad (3)$$

where $\phi^a=(x,q_1,\ldots,q_N,p,k_1,\ldots,k_N)$, $a=1,\ldots,2N+2$, and $\omega^{ab}=-\omega^{ba}$ is the element of the $(2N+2)\times(2N+2)$ symplectic matrix.

The time evolution of classical phase-space probability distribution function of the system plus the bath $P(\phi,t)$ is governed by the following Liouville equation:

$$\dot{P}(\phi,t)=\{P,H\}_{\rm PB}\ , \quad (4)$$

where $\{\ \}_{\rm PB}$ is the Poisson bracket. The formal solution of (4) is

$$P(\phi_f,t)=\int d^{2N+2}\phi_i\delta^{2N+2}[\phi_f^a-\phi_{\rm cl}^a(t,\phi_i)]P(\phi_i,0)\equiv\int d^{2N+2}\phi_i J(\phi_f,t|\phi_i,0)P(\phi_i,0)\ , \quad (5)$$

where $\phi_{\rm cl}^a(t,\phi_i)$ is a classical path that satisfies Hamilton's equation (3) with initial conditions $\phi_{\rm cl}^a(0)=\phi_i^a$. $J(\phi_f,t|\phi_i,0)$ is defined as the conditional probability of the system plus the bath.

Following the work done by Gozzi, Reuter, and Thacker [11], we rewrite the conditional probability (5) in the form of the *path integral of classical mechanics,*

$$J(\phi_f,t|\phi_i,0)=\int D^{2N+2}\phi\int D^{2N+2}\lambda\int D^{2N+2}c\times\int d^{2N+2}\bar{c}\exp\left[i\int_0^t ds\tilde{L}\right]\ , \quad (6)$$

subject to the boundary conditions,

$$\phi^a(0)=\phi_i^a,\quad \phi^a(t)=\phi_f^a\ . \quad (7)$$

In (6), $\lambda_a(s)$ are $2N+2$ auxiliary dynamical variables. We also have introduced $2N+2$ Grassman variables $c^a(s)$ and their conjugates $\bar{c}_a(s)$. These Grassman variables are called ghost fields in field theory. The generalized Lagrangian $\tilde{L}$ in (6) is

$$\tilde{L}=\lambda_a(s)\{\dot{\phi}^a(s)-\omega^{ab}\partial_b H[\phi]\}+i\bar{c}_a(s)\{\delta_b^a\partial_s-\omega^{ac}\partial_c\partial_b H[\phi]\}c^b(s)\ . \quad (8)$$

We note the following identity [11]:

$$\int D^{2N+2}c\int D^{2N+2}c\times\exp\left\{i\int_0^t ds\,i\bar{c}_a\{\delta_b^a\partial_s-\omega^{ac}\partial_c\partial_b H[\phi]\}c^b(s)\right\}=1\ , \quad (9)$$

which implies that the ghost field part of the path integral in (6) can be neglected.

Since we are only interested in the dynamics of the Brownian particle, we define the reduced phase-space probability distribution function for the Brownian particle alone,

$$P_r(x,p,t)=\prod_n\int_{-\infty}^{+\infty}dq_n\times\int_{-\infty}^{+\infty}dk_n P(x,q_1,\ldots,q_N,p,k_1,\ldots,k_N,t)\ . \quad (10)$$

If we assume that at $t=0$ the system and the bath are uncorrelated,

$$P(x,q_1,\ldots,q_n,p,k_1,\ldots,k_n,0)\equiv P_r(x,p,0)P_b(q_1,\ldots,q_N,k_1,\ldots,k_N,0)\ , \quad (11)$$

then

$$P_r(x_f,p_f,t)=\int_{-\infty}^{+\infty}dx_i\int_{-\infty}^{+\infty}dp_i J_r(x_f,p_f,t|x_i,p_i,0)P_r(x_i,p_i,0)\ , \quad (12)$$

where the reduced conditional probability for the Brownian particle is

$$J_r(x_f,p_f,t|x_i,p_i,0)$$
$$=\int_{x_i}^{x_f}Dx\int_{p_i}^{p_f}Dp\int D\lambda_x\int D\lambda_p\exp\left\{i\int_0^t ds\,\lambda_x(s)\left[\dot{x}(s)-\frac{p(s)}{M}\right]+i\int_0^t ds\,\lambda_p(s)[\dot{p}(s)+V'(x)]\right\}F[x,p,\lambda_x,\lambda_p]\ . \tag{13}$$

The *classical influence functional* $F[x,p,\lambda_x,\lambda_p]$ in (13) is

$$F[x,p,\lambda_x,\lambda_p]=\prod_n\int_{-\infty}^{+\infty}dq_{nf}\int_{-\infty}^{+\infty}dk_{nf}\int_{-\infty}^{+\infty}dq_{ni}\int_{-\infty}^{+\infty}dk_{ni}\left[\frac{\beta\omega_n}{2\pi}\right]\exp\left\{-\beta\left[\frac{k_{ni}^2}{2m_n}+\frac{1}{2}m_n\omega_n^2q_{ni}^2\right]\right\}\int_{q_{ni}}^{q_{nf}}Dq_n\int_{k_{ni}}^{k_{nf}}Dk_n$$
$$\times\int D\lambda_{q_n}\int D\lambda_{k_n}\exp i\int_0^t ds\left\{\lambda_{q_n}(s)\left[\dot{q}_n(s)-\frac{k_n(s)}{m_n}\right]+\lambda_{k_n}(s)[\dot{k}_n(s)+m_n\omega_n^2q_n(s)+C_nx(s)]+\lambda_p(s)C_nq_n(s)\right\}, \tag{14}$$

where we assume the bath is at thermal equilibrium with temperature T so the Maxwell-Boltzmann distribution has been used. Performing the path integral in (14) and using the classical trajectory of bath oscillator $q_n(s)_{\rm cl}$ and $k_n(s)_{\rm cl}$, we obtain

$$F[x,p,\lambda_x,\lambda_p]=\exp\left[-\tfrac{1}{2}\int_0^t ds_1\int_0^t ds_2\lambda_p(s_1)\nu(s_1-s_2)\lambda_p(s_2)+2i\int_0^t ds_1\lambda_p(s_1)\int_0^{s_1}ds_2\eta(s_1-s_2)x(s_2)\right], \tag{15}$$

where

$$\nu(s)=2kT\gamma(s) \tag{16}$$

is the noise kernel, and

$$\eta(s)=(d/ds)\gamma(s)\ , \tag{17}$$

where

$$\gamma(s)=\int_0^{+\infty}\frac{d\omega}{\pi}\frac{I(\omega)}{\omega}\cos\omega s \tag{18}$$

is the dissipation kernel. Thus the first term in (15) is the noise term and second term is the dissipation term. The dissipation spectral density $I(\omega)$ in (18) is

$$I(\omega)=\sum_n\frac{\pi C_n^2}{2m_n\omega_n}\delta(\omega-\omega_n)\ , \tag{19}$$

which only depends on the properties of the bath (the bath harmonic-oscillator number density and coupling constants). This spectral density fully determines the properties of the noise and dissipation kernels, and therefore the properties of the Brownian dynamics.

Substituting the classical influence functional (15) into the reduced conditional probability (13) and performing the path integral for $\lambda_x(s)$ and $p(s)$ only gives

$$J_r(x_f,p_f,t|x_i,p_i,0)=\int_{x_i,p_i}^{x_f,p_f}Dx\int D\lambda_p\exp\left[-\tfrac{1}{2}\int_0^t ds_1\int_0^t ds_2\lambda_p(s_1)\nu(s_1-s_2)\lambda_p(s_2)\right]$$
$$\times\exp\left[i\int_0^t ds_1\lambda_p(s_1)\left[M\ddot{x}(s_1)+2\int_0^{s_1}ds_2\eta(s_1-s_2)x(s_2)+V'(x)\right]\right]\ . \tag{20}$$

The boundary conditions for path $x(s)$ denote $x(0)=x_i$ and $\dot{x}(0)=p_i/M$, $x(t)=x_f$ and $\dot{x}(t)=p_f/M$. It is clear that the above classical influence corresponds to the following generalized Langevin equation:

$$M\ddot{x}(s)=-V'(x)-2\int_0^s ds'\eta(s-s')x(s')+\lambda_p(s)\ , \tag{21}$$

and the auxiliary variable $\lambda_p(s)$ is just a Gaussian colored noise source which has the following moments:

$$\langle\lambda_p(s)\rangle=0,$$
$$\langle\lambda_p(s_1)\lambda_p(s_2)\rangle=\nu(s_1-s_2)\equiv2kT\gamma_0(s_1-s_2)\ . \tag{22}$$

It is actually the well-known classical fluctuation-dissipation relation [14].

Finally we perform the path integral over $\lambda_p(s)$ in (20) to obtain the path-integral formulation of classical Brownian motion in a general environment,

$$J_r(x_f,p_f,t|x_i,p_i,0)=\int_{x_i,p_i}^{x_f,p_f}Dx\exp\left[-\tfrac{1}{2}\int_0^t ds_1\int_0^t ds_2Q(s_1)\nu^{-1}(s_1-s_2)Q(s_2)\right], \tag{23}$$

where

$$Q(s)=M\ddot{x}(s)+2\int_0^s ds'\eta(s-s')x(s')+V'(x)\ , \tag{24}$$

and $\nu^{-1}(s)=(\beta/2)\gamma^{-1}(s)$ is the inverse of $\nu(s)$.

This path-integral formalism could be applied to many nonequilibrium statistical physics problems. In many physics applications, an important class of dissipation spectral densities [15] is

$$I(\omega)=\gamma_0\omega(\omega/\tilde{\omega})^se^{-(\omega^2/\Lambda^2)}\ , \tag{25}$$

where γ_0 is the damping constant and $\tilde{\omega}$ is a frequency scale usually taken to be the cutoff frequency Λ. An environment is classified as Ohmic $I(\omega)\sim\omega$ with $(s=0)$, supra-Ohmic $I(\omega)\sim\omega^{1+s}$, $s>0$, or sub-Ohmic $-1<s<0$. In general, the dissipation kernel $\gamma(s)$ is not a δ function, so the dissipation force contains a memory function. From the fluctuation-dissipation relation (22), the noise kernel is also a nonlocal kernel, so the noise is colored.

The most studied case is the Ohmic environment

($s=0$) which induces a dissipative force linear in the velocity of the Brownian particle provided the cutoff frequency Λ is very large. In this special case, $I(\omega)=\gamma_0\omega$, so that $\gamma(s)=\gamma_0\delta(s)$ and $\nu^{-1}(s)=(1/2\gamma_0 kT)\delta(s)$; consequently we get

$$J_r(x_f,p_f,t|x_i,p_i,0)$$

$$=\int_{x_i,p_i}^{x_f,p_f}Dx\exp\left[-\frac{1}{4\gamma_0 kT}\int_0^t ds[M\ddot{x}(s)+\gamma_0\dot{x}(s)+V'(x)]^2\right], \quad (26)$$

which is the result given by Dykman and co-workers [5].

We close this letter with a few general remarks. First, this path-integral formalism of classical Brownian motion in a general environment is exact. It is derived from the first principles of microdynamics. The only assumption is that the Brownian particle and its environment are not correlated at the initial time $t=0$. Further generalization of these results to cases where the Brownian particle and its environment are correlated initially is possible.

Second, this path-integral formalism can be immediately generalized to nonlinearly coupled cases. If the coupling term in the Hamiltonian (2) is $C_n q_n f(x)$, then one can replace $x(s)$ in the dissipation term in (15) by $f(x(s))$ and replace $\lambda_p(s)$ by $f'(x)\lambda_p(s)$ in both the dissipation and noise terms. This corresponds to a nonlinear (nonlocal) damping force in the classical Langevin equation and to nonlinearly coupled colored noise (multiplicative noise). However, the classical fluctuation-dissipation relation for the nonlinear case is still exactly the same as for the linear case (22) [9]. The problem of nonlinear damping and multiplicative noise has important applications in many branches of physics [2].

Third, the dissipation kernel (18) and the dissipation spectral density (19) are exactly the same as the corresponding terms in the quantum influence functional. The noise kernel (16) and the fluctuation-dissipation relation (22) are the same as the corresponding terms of the quantum influence functional at *high temperature* [9]. This is expected since the classical theory is the high-temperature limit of the quantum theory. The proof of this correspondence between quantum and classical influence-functional theories of Brownian motion and details of the present study will be presented elsewhere [16].

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