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LETTER TO THE EDITOR

On the path integral formulation of Brownian dynamics

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Abstract. The path integral formulation of Brownian motion in an external force is reconsidered and a new representation is derived.

Several authors (Wiegel 1986, Langouche *et al* 1979) considered the formulation of the diffusion of a Brownian particle under an arbitrary force by means of path integrals. Their formulation, however, is not convenient for practical calculations. In this letter we will re-examine the approach of these authors and derive a new path-integral representation of the transition probability for a Brownian particle under an arbitrary external force.

The probability density $P(x, t, 0, 0)$ obeys the equation

$$\partial_t P = D_0 \Delta P + D_0 \nabla_x (F(x) P) \tag{1}$$

where D_0 is the diffusion coefficient and $F(x)$ is the force. The transition probability $P(x, t, x', t')$ $(t > t')$ possesses the Markovian property

$$P(x, t, 0, 0) = \int \mathrm{d}x' P(x, t, x', t') P(x', t', 0, 0). \tag{2}$$

For small $t - t'$, $P(x, t, x', t')$ is given by

$$P(x, t, x', t') = \int \mathrm{d}^d p \exp(\mathrm{i}p(x - x') - \mathrm{i}(t - t') h(p, x')) \tag{3}$$

where the Hamiltonian $h(p, x')$ is

$$h(p, x) = -\mathrm{i} D_0 p^2 - D_0 p^\mu F^\mu(x) \tag{4}$$

and d is the space dimension.

After carrying out the integration over p in (3) we obtain

$$P(x, t, x', t') = (4\pi D_0(t - t'))^{-d/2} \exp(-1/(4D_0(t - t'))(x - x' + (t - t') D_0 F(x'))^2). \tag{5}$$

In order to obtain the path-integral representation of the transition probability $P(x, t, 0, 0)$, we divide the interval $(0, t)$ in n intervals $\Delta t = t/n$ and use $n - 1$ times the formula (2). Using (3) and (4) leads respectively to the functional integral in the phase space (Langouche *et al* 1979) and configurational space. The continuous representation of $P(x, t, 0, 0)$ in the configurational space is

$$P(x, t, 0, 0) = \int_{x(0)=0}^{x(t)=x} \mathrm{D}x(t) \exp\left(-(1/4D_0) \int_0^t \mathrm{d}t'(\dot{x}(t') + D_0 F(x(t')))^2\right). \tag{6}$$

Equation (6) has to be understood as an abbreviation of the n-times integral. We notice that the force on the interval (t_{k-1}, t_k) must be taken at the beginning of the interval. The function $P(x, t, x', t')$ given by (5) obeys the equation

$$\partial_t P = D_0 \partial^2 P/\partial x^2 + D_0 \partial_x (F(x')P). \tag{7}$$

With the aid of (6) and (7) one can show that $P(x, t, 0, 0)$ obeys the equation (1).

One can come to the idea of transforming the cross-term in the exponential of (5) as follows

$$(x - x')F(x') = U(x) - U(x') \tag{8}$$

where $F(x) = \partial_x U$. This transform is legitimate in the function theory when $x - x'$ is infinitesimal. Using (8) we can check that for small $t - t'$, $P(x, t, x', t')$ will obey the equation

$$\partial_t P = D_0 \partial^2 P/\partial x^2 + D_0 \partial_x (F(x)P) - (1/2) D_0 \operatorname{div} F(x) P. \tag{9}$$

To avoid the appearance of the last term in (9) instead of (5) we have to use the expression

$$\begin{aligned} P(x, t, x', t') &\\ = (4\pi D_0(t - t'))^{-d/2} &\exp\{-[1/(4D_0(t - t'))(x - x')^2 \\ &- \tfrac{1}{2}(U(x) - U(x')) - \tfrac{1}{4} D_0 (t - t') F(x')^2 \\ &+ \tfrac{1}{2} D_0 (t - t') \operatorname{div} F(x')]\}. \end{aligned} \tag{10}$$

Therefore, we see that instead of (8) we must use the following formula:

$$U(x) - U(x') = (x - x')F(x') + D_0(t - t') \operatorname{div} F(x'). \tag{11}$$

We note that (11) reminds us of the Ito calculus of the stochastic variables (Gardiner 1985).

Analogous to the above the combination of (10) and (2) leads to the path integral representation of $P(x, t, 0, 0)$ discussed by Wiegel (1986).

Because the exponential in (6) is not linear in $F(x)$, the path integral (6) is not convenient for carrying out the perturbative calculations. In order to transform (6) we could use the discretised version of it and expand (6) in powers of the force. But the simplest way is to use the propagator method (Björken and Drell 1965). The differential equation (1) can be rewritten in an integral form as follows

$$P(x, t, 0, 0) = P_0(x, t, 0, 0) + \int_0^t \mathrm{d}t' \int \mathrm{d}x' P_0(x, t, x', t') \nabla_{x'} D_0 F(x') P(x', t', 0, 0) \tag{12}$$

where $P_0(x, t, 0, 0)$ is the Green function of the diffusion equation without the force. The iteration of (12) generates the perturbation expansion of $P(x, t, 0, 0)$ in powers of the force. In each order of this expansion we go from the ordered time integration to the symmetrical one. Thereafter it is easy to see that the perturbation expansion can be represented as

$$P(x,t,0,0)=\int_{x(0)=0}^{x(t)=x} \mathrm{D}x(t)\exp\left(-1/(4D_0)\int_0^t \mathrm{d}t'\,\dot{x}(t')^2+D_0\int_0^t \mathrm{d}t'\,\nabla^\mu F_\mu(x(t'))\right). \quad (13)$$

Equation (13) is a symbolic expression and has to be undertstood in the sense of the perturbation expansion. The derivative in the exponential of (13) acts not only on $F(x(t'))$ but also on the function that appears on the right of F. The second term in the exponential of (13) can be transformed to $-D_0\int_0^t \mathrm{d}t'\,\overleftarrow{\nabla}^\mu F_\mu(x(t'))$, where the nabla, $\overleftarrow{\nabla}^\mu$, acts on the left.

The expression (13) is the main result of the present letter. Let us outline how it follows from (6). As we mentioned above, (6) has to be understood as an n-times integral with a definite prescription of the discretisation. The time integral in the exponential becomes a sum. We look for the Taylor expansion of the term

$$\sum_m (x_m-x_{m-1})F(x_{m-1}). \quad (14)$$

This term appears in combination with the function

$$P_0(x_m-x_{m-1},\Delta t)=(4\pi D_0\Delta t)^{-d/2}\exp(-1/(4D_0\Delta t)(x_m-x_{m-1})^2).$$

Both terms can be represented as follows:

$$P_0(x_m-x_{m-1},\Delta t)2D_0\Delta t\overleftarrow{\nabla}_{x_{m-1}}F(x_{m-1})$$

which agrees with (13). It is easy to see that the square of (14) with $m=n$ compensates for the term $\Sigma_m F(x_{m-1})^2$ in the exponential of (6). An analogous consideration of high-order terms enables one to check that (6) and (13) are equivalent.

In this letter we have derived a new path-integral representation for Brownian motion under an external force. It is remarkable that the exponential of (13) is linear in the force. The simplicity of (13) in comparison with (6) makes it more convenient for practical calculations, especially for the perturbative ones. Equation (13) is convenient in the case when the force is a stochastic one and the average over it is necessary.

Assuming that the distribution of the random force $F^\mu(x)$ is given by the Gauss law with the correlation function

$$\langle F^\mu(x)F^\nu(x')\rangle=C^{\mu\nu}(x-x')$$

we obtain from (13)

$$P(x,t,0,0)=\int_{x(0)=0}^{x(t)=x} \mathrm{D}x(t)\exp\left(-1/(4D_0)\int_0^t \mathrm{d}t'\,\dot{x}(t')^2+\tfrac{1}{2}\int_q a^\mu(q)a^\nu(-q)C^{\mu\nu}(q)\right) \quad (15)$$

where $a^\mu(q)=D_0\int_0^t \mathrm{d}t'\,\overleftarrow{\nabla}^\mu_{x(t')}\mathrm{e}^{\mathrm{i}qx(t')}$ and $\int_q=\int \mathrm{d}^dq/(2\pi)^d$. The exact linearity of the exponential of (13) in F enabled us to carry out the average over the random force. Equation (15) enables one to investigate the random walk in a random environment. It is easy to see that the perturbation expansion of (15) in powers of $C^{\mu\nu}(q)$ can be represented by means of diagrams. Equation (15) can be considered as an alternative to the (field-theoretic) methods used by Fisher (1984), Fisher *et al* (1985), Kravtsov *et al* (1985), and Honkonen and Karjalainen (1988).

The application of (15) to the study of the drift of a Brownian particle in a random environment when an additional constant force acts on the particle is in work (Stepanow 1990). In this case we have to exchange $\dot{x}(t)$ in (15) in accordance to (6) by $\dot{x}(t)+D_0F$. The using of (15) enables one to avoid the replica trick in calculating the mean square displacement of the Brownian particle in a random environment.

An interesting application of (13) and (15), which is currently under study, is the diffusion of a polymer chain in a random environment. A similar problem has been addressed by Muthukumar and Baumgärtner (1989) with the aid of Monte Carlo simulations.

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