Small-fluctuation expansion of the transition probability for a diffusion process

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In many applications of diffusion processes, fluctuations can be considered as a small perturbation of the underlying deterministic dynamics. These situations are currently believed to be described by an asymptotic expansion of the corresponding transition probability in powers of the (small) diffusion coefficient. We offer a systematic procedure whereby *all* further terms in the above expansion can be *systematically* computed in terms of the solutions to certain Lagrange equations associated with the underlying deterministic dynamics.

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Diffusion processes find many important applications in several fields of research, like mesoscopic physics, quantum optics, chemical reaction theory, and population dynamics. We all know that these processes are fully described by the *probability density* $P(x,t)$ and the *transition probability* (density) $P(x,t|x_0,t_0)$ $(t \geq t_0)$. Moreover, we recall that a diffusion process can be viewed as a deterministic first-order time evolution—defined by the *drift velocity* field $V(x,t)$—perturbed by Gaussian fluctuations parametrized by the *diffusion coefficient* D (assumed throughout constant) [1]. As a consequence, $P(x,t)$ obeys the Fokker-Planck equation [2]

$$\frac{\partial}{\partial t}P(x,t)=D\nabla^2 P(x,t)-\frac{\partial}{\partial x_i}[V_i(x,t)P(x,t)] \tag{1}$$

whereas $P(x,t|x_0,t_0)$ is its *fundamental solution* (propagator). Actually, the latter object enjoys the functional integral representation [3,4]

$$P(x'',t''|x',t')=\int \mathcal{D}x(t)\delta(x''-x(t''))\delta(x'-x(t'))\exp\left\{-(1/2D)\int_{t'}^{t''}dt\,L(x(t),\dot{x}(t),t)\right\}, \tag{2}$$

in which $L(x,\dot{x},t)$ is the so-called Wiener-Onsager-Mahlup Lagrangian:

$$L(x,\dot{x},t)\equiv L_0(x,\dot{x},t)+D\frac{\partial}{\partial x_i}V_i(x,t)\equiv\tfrac{1}{2}[\dot{x}_i-V_i(x,t)]^2+D\frac{\partial}{\partial x_i}V_i(x,t)\ . \tag{3}$$

Quite often (in the above-mentioned applications) fluctuations are a small perturbation of the deterministic dynamics, and so looking for *exact* solutions to Eq. (1)—equivalently, carrying out the *exact* path summation in Eq. (2)—becomes an unnecessary task. Rather, it is sufficient to find *asymptotic solutions* of Eq. (1) in the limit of *small D*. As it turns out, the first step toward this goal is more easily accomplished by evaluating the path integral (2) in the same limit. Basically, this amounts to performing a saddle-point expansion in Eq. (2), which gives to lowest order in D [3]

$$P(x'',t''|x',t')\simeq(4\pi D)^{-N/2}[J(x'',t'';x',t')]^{1/2}\exp\{-[Z(x'',t'';x',t')+W_0(x'',t'';x',t')/2D]\}\ , \tag{4}$$

with

$$W_0(x'',t'';x',t')\equiv\int_{t'}^{t''}dt\,L_0(x,\dot{x},t)|_{x=q(t;x'',t'';x',t')}\ , \tag{5a}$$

$$Z(x'',t'';x',t')\equiv\frac{1}{2}\int_{t'}^{t''}dt\frac{\partial}{\partial x_i}V_i(x,t)|_{x=q(t;x'',t'';x',t')}\ , \tag{5b}$$

where $q(t;x_2,t_2;x_1,t_1)$ denotes the solution of the Lagrange equations stemming from $L_0(x,\dot{x},t)$, which goes through both (x_1,t_1) and (x_2,t_2), while $J(x_2,t_2;x_1,t_1)$ is the *Van Vleck determinant* [5] associated with $W_0(x_2,t_2;x_1,t_1)$.

However, all this is not the end of the story, for Eq. (4) merely yields the first of infinitely many terms in the asymptotic expansion of the transition probability.

Our aim is to provide a strategy that permits the *systematic evaluation* of higher-order corrections to Eq. (4) in the limit of small diffusion coefficient. As we shall see, the resulting complete asymptotic expansion of $P(x'',t''|x',t')$ is fully expressed in terms of the previously introduced deterministic trajectory $q(t;x_2,t_2;x_1,t_1)$.

Our result can be most neatly stated with the help of some preliminary definitions. Denoting by $f(x)$ a smooth arbitrary function, we introduce the following second-order differential operator:

$$\hat{\Omega}(x,t;x',t')f(x)\equiv[J(x,t;x',t')]^{-1/2}\nabla_x^2\{[J(x,t;x',t')]^{1/2}f(x)\}-2\frac{\partial Z(x,t;x',t')}{\partial x_i}\frac{\partial}{\partial x_i}f(x)$$
$$+\left[\left[\frac{\partial Z(x,t;x',t')}{\partial x_i}\right]^2-\frac{1}{J(x,t;x',t')}\frac{\partial}{\partial x_i}\left[J(x,t;x',t')\frac{\partial Z(x,t;x',t')}{\partial x_i}\right]\right]f(x)\ . \qquad (6)$$

Moreover, we define recursively

$$\mathcal{B}_n(x,t;x',t';t_1,\ldots,t_n)\equiv\hat{\Omega}(x_n,t_n;x',t')\mathcal{B}_{n-1}(x_{n-1},t_{n-1};x',t';t_1,\ldots,t_{n-1})|_{x_n=q(t_n;x,t;x',t')}\ , \qquad (7)$$

with $\mathcal{B}_0\equiv 1$, and

$$b_n(x,t;x',t')\equiv\int_{t'}^{t}dt_n\ldots\int_{t'}^{t_2}dt_1\mathcal{B}_n(x,t;x',t';t_1,\ldots,t_n)\quad(n\geq 1)\ , \qquad (8)$$

while it is understood that $b_0\equiv 1$. Then the full asymptotic expansion of $P(x'',t''|x',t')$ is given by

$$P(x'',t''|x',t')_{\rm asym}=(4\pi D)^{-N/2}[J(x'',t'';x',t')]^{1/2}$$
$$\times\exp\{-[Z(x'',t'';x',t')+W_0(x'',t'';x',t')/2D]\}\sum_{n=0}^{\infty}D^n b_n(x'',t'';x',t')\ . \qquad (9)$$

A study of the very difficult question concerning the convergence of Eq. (9) goes far beyond the scope of the present paper, although experience with similar problems [6] suggests that the series in Eq. (9) is in general a divergent asymptotic one.

The proof of Eq. (9)—though not particularly difficult—would be too long to be reported here. So, we shall merely sketch its basic steps. Briefly, it makes use of the following well-known results about the classical dynamics defined by Lagrangian $L_0(x,\dot{x},t)$: (i) $W_0(x,t;x',t')$ obeys (in the x,t variables) the Hamilton-Jacobi equation associated with $L_0(x,\dot{x},t)$; (ii) $q(t;x'',t'';x',t')$ is just the solution of the first-order equation

$$\frac{d}{dt}q_i(t)=\left[\frac{\partial}{\partial x_i}W_0(x,t;x',t')+V_i(x,t)\right]\Bigg|_{x=q(t)} \qquad (10)$$

as selected by the initial condition $q(t'')=x''$; (iii) the Van Vleck determinant $J(x,t;x',t')$ satisfies (in the x,t variables) the continuity equation associated with Eq. (10); (iv) as a consequence of Eq. (10), the following equation holds true [7]:

$$\frac{\partial}{\partial t}q_i(t_*;x,t;x',t')+\left[\frac{\partial}{\partial x_j}W_0(x,t;x',t')+V_j(x,t)\right]$$
$$\times\frac{\partial}{\partial x_j}q_i(t_*;x,t;x',t')=0\ . \qquad (11)$$

Now, a natural ansatz for $P(x'',t''|x',t')_{\rm asym}$ is just Eq. (9), where at this stage the functions $b_n(x'',t'';x',t')$ are of course unknown (their determination is in fact our present goal). Obviously, consistency with Eq. (4) implies $b_0=1$ and the request that Eq. (9) should obey the (initial time normalization) condition $P(x'',t'|x',t')_{\rm asym}=\delta(x''-x')$ demands

$$b_n(x'',t';x',t')=0\ ,\quad n\geq 1 \qquad (12)$$

since Eq. (4) already meets such a condition. We proceed by inserting Eq. (9)—with x'',t'' replaced by x,t—into Eq. (1). Thanks to the above-mentioned (i), (iii), and (iv) facts, the following *transport equations* for the unknown functions $b_n(x,t;x',t')$ arise (after various arrangements)

$$\left[\frac{\partial}{\partial t}+\left[\frac{\partial}{\partial x_i}W_0(x,t;x',t')+V_i(x,t)\right]\frac{\partial}{\partial x_i}\right]b_n(x,t;x',t')$$
$$=\hat{\Omega}(x,t;x',t')b_{n-1}(x,t;x',t')\ . \qquad (13)$$

As a matter of fact, Eq. (13) can be solved easily. Perhaps, the simplest procedure consists in first setting $x=q(t;x'',t'';x',t')$ in Eq. (13). Because of Eq. (10), the left-hand side of the resulting equations is then recognized as the total time derivative of $b_n\{q(t;x'',t'';x',t'),t;x',t'\}$. Hence, we find by integration [using Eq. (12)]

$$b_n(x'',t'';x',t')=\int_{t'}^{t''}dt\,\hat{\Omega}(x,t;x',t')$$
$$\times b_{n-1}(x,t;x',t')|_{x=q(t;x'',t'';x',t')}\ . \qquad (14)$$

On account of $b_0=1$ and Eqs. (7), repeated use of Eq. (14) precisely gives Eq. (8). Q.E.D.

Before closing this paper, a comment is in order. Any normalizable function defined over an infinite range should necessarily vanish at infinity. Now—thanks to the structure of Eq. (1)—any solution $P(x,t)$ of that Fokker-Planck equation that vanishes for any t at spatial infinity together with $\nabla P(x,t)$ remains normalized, if it was so at some initial time. Applying this result to Eq. (9), we conclude that $P(x'',t''|x',t')_{\rm asym}$ is indeed normalized to one for any $t''>t'$ (since it is at t') provided the above boundary conditions are fulfilled.

Details about the matter discussed in the present paper and illustrative examples will be reported elsewhere.

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[1] We shall be concerned throughout with diffusion processes occurring in N-dimensional configuration space $\mathbb{R}^N$. So, x should be understood as a vector in $\mathbb{R}^N$ and the index i (see below) runs from 1 to N. Repeated indices are summed over.

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[4] Equation (2) is supposed to be defined by means of the midpoint time-slicing discretization. This circumstance is responsible for the divergence of the drift in Eq. (3) [3] and implies that the action integral in Eq. (2) has to be understood in the sense of Stratonovich [2].

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[7] Equation (11) can be derived by the same reasoning that leads to Eq. (10) of F. Guerra and L. Morato, Phys. Rev. D **27**, 1774 (1983).