High-accuracy discrete path integral solutions for stochastic processes with noninvertible diffusion matrices

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The derivation of the discrete path integral solution for the propagator is known to present a special problem for those stochastic processes whose diffusion matrices are noninvertible. In this paper two methods for formulating the stochastic dynamics in terms of path integrals are developed that are applicable whether or not the diffusion matrix is invertible. One of the methods is an extension of the standard technique available for the derivation of the functional formalism from Langevin equations. An accurate discretization scheme is used to replace these equations by finite-difference equations and a short time approximation for the propagator is then derived in terms of known statistical properties of noise terms. An alternative derivation of the discrete path integral is presented in terms of the Fokker-Planck formulation without the necessity of introducing discretization schemes into the discussion. This is achieved by making use of the cumulant generating function which is different in this realm. The mutual correspondence of the methods is established and their possible extensions are discussed. Both methods are indeed rigorous and allow for the *systematic* derivation of the short time propagator valid to any desired precision in a time increment τ. Its use in a path integral means a significant reduction of the number of time steps that are required to achieve a given level of accuracy for a given net increment $t=N\tau$, and, therefore, significantly increasing the feasibility of path integral calculations. Another attractive feature of the present techniques is that they permit the efficient treatment of equations with singular diffusion matrices, two of which, a Kramers equation and a colored-noise problem, are considered. [S1063-651X(97)08403-1]

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I. INTRODUCTION

The analysis and understanding of dynamical phenomena remains one of the fundamental goals of physics. In particular, considerable effort has been recently devoted to studying realistic systems driven by noise and friction. It is known that the statistical dynamics of such systems can be described in a formally equivalent way by following either the Fokker-Planck equation

$$\partial_t P(\mathbf{q},t)=LP(\mathbf{q},t)\equiv[-\partial_i G_i(\mathbf{q})+\tfrac{1}{2}\partial_{ij}^2 D_{ij}(\mathbf{q})]P(\mathbf{q},t) \tag{1}$$

or a set of Langevin equations,

$$\dot{\mathbf{q}}(t)=\mathbf{G}[\mathbf{q}(t)]+\mathbf{B}[\mathbf{q}(t)]\mathbf{F}(t), \tag{2}$$

with $\mathbf{F}^T(t)=\{F_1(t),\ldots,F_m(t)\}$ being Gaussian white noise normalized to

$$\langle F_i(t)\rangle=0, \quad \langle F_i(t)F_j(s)\rangle=\delta_{ij}\delta(t-s), \tag{3}$$

wherein the standard summation convention over repeated indexes is implied, while the dot denotes the time derivative. Although the systematic variables $\mathbf{q}^T=\{q_1,\ldots,q_m\}$ of Eq. (1) are generally different from the stochastic variables $\mathbf{q}^T(t)=\{q_1(t),\ldots,q_m(t)\}$ governed by Eq. (2), we do not distinguish them notationally to keep the presentation simple. One also notes here that there is a connection between the Fokker-Planck coefficients **G** and **D** and those of Eq. (2). It depends upon the interpretation of the stochastic integral

$$\int_0^t ds\ \mathbf{B}[\mathbf{q}(s)]\mathbf{F}(s), \tag{4}$$

but this point will be discussed at greater length in Sec. II.

The Fokker-Planck and Langevin equations, firstly applied to investigate Brownian motion [1] and the diffusion model of chemical reactions [2,3], are now largely employed, in various generalized forms, in many fields involving stochastic processes. General reviews have recently been given by Gardiner [4] and Risken [5]. As it is generally not possible to obtain closed form analytical solutions of second-order partial differential equations, many successful numerical schemes have been developed during the last decade, which integrate the Fokker-Planck equation on a grid [6,7] or in a basis set [8]. Their utility, however, is strongly limited by the storage requirements and execution time that grow very rapidly with the dimensionality of the system under study. With present day computers, exact schemes are feasible in practice for systems of a few degrees of freedom, while truly multidimensional systems are usually dealt with using approximate techniques. Computer simulation of Langevin equations is not so restrictive with respect to the dimensionality and could be very accurate with intensive computational efforts [9,10]. The numerical schemes available for the integration of these equations are computationally efficient in terms of storage requirements; but they become ineffective and may even give false results when

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dealing with systems with more than one stable state, for which simulations over very long-time lengths are usually required [11]. The various approximate methods could also be employed for analytically treating Fokker-Planck and Langevin equations, provided that their specific assumptions are satisfied.

Among the rest of the methods substantial attention has been given to the path integral representation of statistical dynamics. This arises very naturally from the context of stochastic processes, and was first studied in detail by Wiener for Brownian motion [12]. Ever since Feynman proposed path integration as an alternative formulation of nonrelativistic quantum mechanics [13], the path integral method has been successfully applied to almost all branches of theoretical physics [14]. The reason for this seems to be the fact that path integrals are often beautiful and elegant answers to physical problems. They are more than solutions of appropriate Schrödinger, Fokker-Planck, or Langevin equations. Their formulations incorporate global properties of the system and they can give answers which are not obvious in terms of partial (or stochastic) differential equations. As a result, the path integral method provides a powerful tool for formal manipulations, for doing both perturbative and nonperturbative, systematic treatments [13–19]. Numerical applications have also become increasingly important during the last decade and have often led to new physical results not obtainable by other means [19,20]. From a computational point of view, the most appealing feature of the method is perhaps that it avoids explicit reference to distribution functions whose storage requirements grow exponentially with the number of coupled degrees of freedom. Instead, all dynamical characteristics are included in a discrete path integral representation of the conditional probability (propagator), which expresses the distribution function for any (arbitrary) time t

$$P(\mathbf{q},t)=\int\prod_{n=0}^{N-1}d\mathbf{q}^n P_{(k)}(\mathbf{q}^{n+1},\tau|\mathbf{q}^n)P(\mathbf{q}^0,0)+O(t^{k+1}/N^k) \tag{5}$$

in terms of the known short time propagator. Hereby, we set $\mathbf{q}^N=\mathbf{q}$, $\tau=t/N$, and introduced the short time propagator $P_{(k)}(\mathbf{q}^{n+1},\tau|\mathbf{q}^n)$ which is an approximation for the true propagator $P(\mathbf{q}^{n+1},\tau|\mathbf{q}^n)$,

$$P(\mathbf{q}^{n+1},\tau|\mathbf{q}^n)=P_{(k)}(\mathbf{q}^{n+1},\tau|\mathbf{q}^n)+O(\tau^{k+1}), \tag{6}$$

valid at least to first order in $\tau,(k=1)$. In practice, though, one would like for the short time propagators to be accurate for an order in τ as high as possible, in order to keep the number of integration variables in Eq. (5) as small as possible (for a given net time increment t).

As there exists no unique way to determine the short time propagator, many different path integrals corresponding to various different approximate schemes have resulted. An extensive review on this subject can be found in Ref. [21]. The most obvious derivation utilizes the usual limiting procedure in which the time interval $[0,t]$ is divided into N equal subintervals $[0,t_1],[t_1,t_2],\ldots,$ of duration τ, and Eq. (2) is replaced by a difference equation

$$\mathbf{q}^{n+1}-\mathbf{q}^n=\int_{t_n}^{t_{n+1}}ds\ \mathbf{G}[\mathbf{q}(s)]+\int_{t_n}^{t_{n+1}}ds\ \mathbf{B}[\mathbf{q}(s)]\mathbf{F}(s), \tag{7}$$

with $\mathbf{q}^n=\mathbf{q}(t_n)$ and $t_n=n\tau$. For simplicity, we restrict ourselves in this section to state-independent matrices B_{ij}. Then, the *result* of the functional representation of the probability $P(\mathbf{q},t)$ is independent of the discretization scheme for the stochastic integral, Eq. (4). That is, the Langevin equation (2) is equivalent to the Fokker-Planck equation (1) with a diffusion matrix $D_{ij}=B_{ik}B_{jk}$, and no problems of the type of the Stratonovich versus Ito interpretation arise in this case [4].

The common procedure relies on the primitive integration scheme (see, e.g., [15,22])

$$\mathbf{q}^{n+1}-\mathbf{q}^n-\tau[\mu\mathbf{G}(\mathbf{q}^{n+1})+(1-\mu)\mathbf{G}(\mathbf{q}^n)]=\mathbf{B}\mathbf{f}^{n+1}, \tag{8}$$

where μ is an arbitrary number from the interval $[0,1]$, while the notation $\mathbf{f}^{n+1}$ stands for

$$\mathbf{f}^{n+1}=\int_{t_n}^{t_{n+1}}ds\ \mathbf{F}(s). \tag{9}$$

Equation (8) relates the two sets of variables $(\mathbf{q}^1,\ldots,\mathbf{q}^N)$ and $(\mathbf{f}^1,\ldots,\mathbf{f}^N)$. The corresponding probabilities of the discretized realization P and R are therefore related by the equation

$$P(\mathbf{q}^N,\ldots,\mathbf{q}^1|\mathbf{q}^0)=R(\mathbf{f}^N,\ldots,\mathbf{f}^1)J(\mathbf{q}^N,\ldots,\mathbf{q}^0), \tag{10}$$

with J being the Jacobian of the transformation $\det[\delta\mathbf{f}/\delta\mathbf{q}]$,

$$\begin{aligned}J&=\det\left(\frac{\partial f_i^n}{\partial q_j^k}\right)\\&=D^{-N/2}\det[\delta_{i,j}\delta_{n,k}-\delta_{i,j}\delta_{n-1,k}-\mu\tau\delta_{n,k}\partial_j G_i(\mathbf{q}^n)\\&\quad-(1-\mu)\tau\delta_{n-1,k}\partial_j G_i(\mathbf{q}^{n-1})],\end{aligned} \tag{11}$$

where $D=\det(D_{ij})=\det^2(B_{ij})$. The Jacobian can be evaluated by using the matrix identity for the determinant [15]

$$\begin{aligned}\det(\mathbf{I}-\mathbf{M})&=\exp[\mathrm{Tr}\ \ln(\mathbf{I}-\mathbf{M})]\\&=\exp[\mathrm{Tr}(-\mathbf{M}-\tfrac{1}{2}\mathbf{M}^2-\cdots)],\end{aligned} \tag{12}$$

which gives to order τ

$$J=\prod_{n=1}^{N}D^{-1/2}\exp[-\mu\tau\partial_i G_i(\mathbf{q}^n)]. \tag{13}$$

The multivariate probability of the variables $\mathbf{f}^n$ is readily determined in terms of the known statistical properties of the random noise $\mathbf{F}(t)$, Eq. (3), to yield

$$R(\mathbf{f}^N,\ldots,\mathbf{f}^1)=\prod_{n=1}^{N}(2\pi\tau)^{-m/2}\exp\left(-\frac{1}{2\tau}|\mathbf{f}^n|^2\right). \tag{14}$$

Then, writing the propagator of the process $\mathbf{q}(t)$ as

$$P(\mathbf{q},t|\mathbf{q}^0)=\int\prod_{n=1}^{N-1}d\mathbf{q}^n P(\mathbf{q}^N=\mathbf{q},\ldots,\mathbf{q}^1|\mathbf{q}^0), \tag{15}$$

one immediately obtains the discrete path integral representation

$$P(\mathbf{q},t)\approx\int\prod_{n=0}^{N-1}d\mathbf{q}^n[(2\pi\tau)^m D]^{-1/2}\exp\Big\{-\tau\mu\partial_i G_i(\mathbf{q}^{n+1})$$
$$-\frac{1}{2\tau}D^{ij}[q_i^{n+1}-q_i^n-\tau\mu G_i(\mathbf{q}^{n+1})$$
$$-\tau(1-\mu)G_i(\mathbf{q}^n)][]_j\Big\}P(\mathbf{q}^0,0), \tag{16}$$

where D^{ij} is the element of the inverse diffusion matrix $\mathbf{D}^{-1}$, while $[]_j$ means the same bracket as in front of it but with the index j instead of i. It is not hard to see that the right-hand side of Eq. (16) is a product of the short time, or single step propagators

$$P_{(1)}(\mathbf{q}^{n+1},\tau|\mathbf{q}^n)=[(2\pi\tau)^m D]^{-1/2}\exp\Big\{-\tau\mu\partial_i G_i(\mathbf{q}^{n+1})$$
$$-\frac{1}{2\tau}D^{ij}[q_i^{n+1}-q_i^n-\tau\mu G_i(\mathbf{q}^{n+1})$$
$$-\tau(1-\mu)G_i(\mathbf{q}^n)][]_j\Big\}, \tag{17}$$

each one propagating the system for time τ. One notes that analogous results can also be obtained in terms of the Fokker-Planck description, e.g., by using the Trotter splitting of the time evolution operator $\exp(tL)$ based on partitioning the Fokker-Planck operator L into drift and diffusion terms [23].

From a purely formal point of view, the existing path integral representations are all equivalent to each other, as they become an equality in the limit $N\to\infty$ (whatever μ). In practice, only a few path integrals can be evaluated exactly in this limit, and the approximate evaluation of Eq. (5) with finite N seems useful and sometimes necessary. Therefore, there can be practical advantages to choosing one path integral representation over the others. When treating path integrals numerically, the obvious criteria for their selection are the ease of implementation and convergence properties. The higher the rate of convergence of a path integral, the smaller the number of time steps (and therefore the execution time) that are required to evaluate it to a given level of accuracy. Until recently, however, the only requirement usually made on the short time propagator was that it satisfies Eq. (1) to order $O(\tau)$.

The problem of importance is thus to develop a systematic theoretical formalism for constructing path integral representations (single step propagators) valid to any desired order in $1/N$ (in τ) which is rigorous and also simple to implement. This problem has been resolved in our earlier papers [21,24] in terms of the Fokker-Planck formulation by expanding the exponent of the propagator in a power series in t,

$$P(\mathbf{q},t|\mathbf{q}^0)=[(2\pi t)^m D]^{-1/2}\exp\Big[-\frac{1}{2t}(\mathbf{q}-\mathbf{q}^0)^T\mathbf{D}^{-1}(\mathbf{q}-\mathbf{q}^0)$$
$$+t^k\mathcal{W}_k(\mathbf{q},\mathbf{q}^0)\Big], \tag{18}$$

where the index of summation varies from 0 to ∞. Integral recursive relations are obtained for the expansion coefficients $\mathcal{W}_k$ which can be *analytically* evaluated in many situations of practical interest. Any finite truncation of the series in Eq. (18) at $k>0$ was shown to be much more accurate than the standard short time approximation (17), allowing for much larger time increments in a path integral. In a recent series of papers [25,26], this formalism has been substantially modified and improved, so that we have managed to deal very efficiently with general Fokker-Planck Schrödinger processes, and their dynamics can now be calculated *accurately* with *any* number of degrees of freedom for *arbitrarily large* times using solely the *single step* propagator.

Two disadvantages of the above mentioned formalism are as follows. The power series expansion for the propagator is efficient if and only if the coefficients of the Fokker-Planck equation $G_i(\mathbf{q})$ and $D_{ij}(\mathbf{q})$ are simple enough (polynomials or a finite sum of exponentials) so that the various integrals involved in $\mathcal{W}_k(\mathbf{q},\mathbf{q}^0)$ are doable analytically. Otherwise, the calculations rapidly become very arduous especially for curved manifolds when the curvature tensor associated with D^{ij} does not vanish. In the latter case we have failed to go beyond $k=1$ [21]. Another disadvantage of the power series expansions formalism, which is also inherent to Eq. (17), is that its utility is restricted to processes with invertible diffusion matrices. But the invertibility of D_{ij} is not a generic case. There is a wide class of physically meaningful stochastic models whose diffusion matrices are noninvertible. The latter property implies that the integration measure for the standard path integral representations available in the literature for multidimensional stochastic processes [see, e.g., Eq. (16)] becomes a singular (δ-function-like) quantity. This makes impossible the numerical evaluation of the path integral and hinders considerably obtaining explicit solutions or approximations of the WKB type.

The above observations inspire the quest for other path integral representations free of these two drawbacks. One might at first believe that this issue should have been settled long ago, namely, because of its continuous usefulness in many problems ranging from chemical physics to biology. Still, a look at textbooks on path integration [14] as well as some recent attempts [15,17,18] in this direction manifestly show that this is *not* the case. To the best of our knowledge, there are no general discrete path integral solutions of such equations other than those derived recently by the present author in terms of an operator decoupling technique [27]. These representations, however, are valid to order N^{-2} solely. Thus, a satisfactory solution to the above-posed problem is *effectively* still lacking.

Our aim is to try to remedy this disappointing situation. The remainder of the paper is organized as follows. In Sec. II we present a straightforward method for the *systematic* derivation of better short time propagators from the Langevin equations (2). By better we mean analytically obtainable, easily evaluateable approximations for the single step propa-

gator accurate for an order in τ as high as possible. An alternative derivation of the discrete path integral is presented in Sec. III. It relies on the Fokker-Planck description of the stochastic dynamics. Numerical applications to an activated rate process in a double well given in Sec. IV show the new single step propagator to be a dramatic improvement over the standard short time approximation. Its use in a path integral means that a given level of accuracy is easily achieved without any increase (or even with a smaller value) of the number of time steps N just due to increasing the order of approximation k. Both approaches are rather general and allow for equations with singular diffusion matrices, two of which, a Kramers equation and a colored-noise problem, are considered. Section V concludes with some general remarks.

II. DISCRETIZATION OF THE LANGEVIN EQUATION

The key idea of the method we present below is the same as in the formal path integral derivation outlined in the Introduction. It consists of two steps. The first step is to obtain an approximate solution, for a short time τ, of the stochastic process $\mathbf{q}(t)$. The second step is the construction of the short time propagator in terms of the known statistical properties of the noise $\mathbf{F}(t)$. The method is combinatorial and does not depend on the dimensionality of the considered process. Therefore we shall illustrate it in the simplest possible situation, that is, a one-dimensional stochastic equation. At the end we shall indicate the obvious steps to adapt the method to nontrivial cases.

More explicitly, the stochastic equation is

$$x(t_n+\tau)=x_n+\int_{t_n}^{t_n+\tau} ds\ G[x(s)]+\int_{t_n}^{t_n+\tau} ds\ B[x(s)]F(s), \tag{19}$$

with

$$\langle F(t)\rangle=0, \quad \langle F(t)F(s)\rangle=\delta(t-s). \tag{20}$$

The common method of approximately solving equations of such the type relies on the expansion of their coefficients in a Taylor series about the prepoint $x_n=x(t_n)$ (see, e.g., Refs. [10] and [28]). The resulting equation is then solved iteratively by using the recurrence relation

$$x_{(k)}(t_n+\tau)=x_n+\sum_{i=0}^{2k-1}\frac{G_n^{(i)}}{i!}\int_{t_n}^{t_n+\tau} ds[x_{(k)}(s)-x_n]^i + \sum_{i=0}^{2k}\frac{B_n^{(i)}}{i!}\int_{t_n}^{t_n+\tau} ds\ F(s)[x_{(k)}(s)-x_n]^i, \tag{21}$$

where $Z_n^{(i)}=[d^iZ(x)dx^i]_{x_n}$, $Z=G,B$. In order to keep the presentation simple, we will not go, in this section, beyond second order in τ. Neglecting terms of an order higher than τ^2, one obtains

$$x_{n+1}-y(x_n,\tau)=u_{n+1}, \tag{22}$$

where the deterministic portion of $x(t)$ reads

$$y(x_n,\tau)=x_n+\tau G_n+\frac{\tau^2}{2}G_nG_n', \tag{23}$$

while the stochastic portion is given after rearranging by

$$\begin{aligned} u_{n+1}=&B_nW_0(\tau)+B_nG_n'W_1(\tau)+\frac{1}{2}B_n^2G_n''\int_0^\tau ds\ W_0^2(s)\\ &+B_n'\Big[B_nI_1(\tau)+G_n\int_0^\tau ds\ F(s)s+B_nG_n'^2\int_0^\tau ds\ I_1(s)\\ &+B_nB_n'\int_0^\tau ds\ F(s)I_1(s)+B_nG_n'\int_0^\tau ds\ F(s)W_1(s)\Big]\\ &+\frac{1}{2}B_n''\Big[B_n^2I_2(\tau)+B_n^2\int_0^\tau ds\ F(s)I_2(s)\\ &+2B_nG_n\int_0^\tau ds\ F(s)W_0(s)s\\ &+2B_n^2B_n'\int_0^\tau ds\ F(s)W_0(s)I_1(s)\Big]+\frac{1}{6}B_n^3B_n'''I_3(\tau). \end{aligned} \tag{24}$$

Hereby, the prime denotes differentiation with respect to x, and the notations W_i and I_i stand for

$$I_i(\tau)=\int_0^\tau ds\ F(s)W_0^i(s),$$

$$W_i(\tau)=\int_0^\tau dt_i\int_0^{t_i}dt_{i-1}\cdots\int_0^{t_2}dt_1\int_0^{t_1}dt_0F(t_0). \tag{25}$$

Equation (22) relates the two sets of variables $(x_N,\ldots,x_1)$ and $(u_N,\ldots,u_1)$. As the functions involved in Eq. (22) are all evaluated at the prepoint x_n, the Jacobian of the transformation is equal to unity in this case. Therefore, the short time propagator of the discretized x realization reads

$$P_{(k)}(x_{n+1},\tau|x_n)=R_{(k)}(u_{n+1},\tau), \tag{26}$$

where R is the probability distribution of the fluctuating term u_{n+1}.

The second step of the present method is thus the derivation of the statistical properties of the noise term. The result of this derivation depends on the interpretation of the various stochastic integrals involved in Eq. (24). Two different interpretations are commonly used. In Ito's interpretation, the integrals I_n are determined by

$$I_i(\tau)=\frac{1}{i+1}W_0^{i+1}(\tau)-\frac{i}{2}\int_0^\tau ds\ W_0^{i-1}(s). \tag{27}$$

While in the Stratonovich interpretation these read

$$I_i(\tau)=\frac{1}{i+1}W_0^{i+1}(\tau). \tag{28}$$

For simplicity we will follow, without loss of generality, Ito's interpretation, in which case a stochastic process obeying Eq. (2) is equivalent to a diffusion process defined by Eq.

(1) with a diffusion matrix $\mathbf{D}(\mathbf{q})=\mathbf{B}(\mathbf{q})\mathbf{B}^T(\mathbf{q})$ [4]. With this choice just a few terms of Eq. (24) contribute to the averages $\langle u_{n+1}^i\rangle$, the first two of which take the form

$$\langle u_{n+1}\rangle=\tfrac{1}{4}\tau^2 B_n^2 G_n'',$$

$$\langle u_{n+1}^2\rangle=M_2(x_n,\tau)=\tau B_n^2+\frac{\tau^2}{2}(2B_n^2G_n'+2G_nB_nB_n'+B_n^2B_n''^2+B_n^3B_n''). \tag{29}$$

Moreover, it is a simple matter to show that all cumulants of higher order than 2 vanish. The latter property implies that the stochastic process u remains Gaussian up to and including terms of order τ^2. This immediately yields

$$P_{(2)}(x_{n+1},\tau|x_n)=[2\pi M_2(x_n,\tau)]^{-1/2}\times\exp\left\{-\frac{[x_{n+1}-M_1(x_n,\tau)]^2}{2M_2(x_n,\tau)}\right\}, \tag{30}$$

where

$$M_1(x_n,\tau)\equiv y(x_n,\tau)+\langle u_{n+1}\rangle=x_n+\tau G_n+\frac{\tau^2}{2}(G_nG_n'+\tfrac{1}{2}B_n^2G_n''), \tag{31}$$

and $M_2(x_n,\tau)$ is defined by Eq. (29). The above derivation is fairly straightforward and can always be continued to any desired order $\tau^k, k>2$. One notes, however, that the stochastic process u is not generally Gaussian for $k>2$, and non-Gaussian corrections are to be included in higher-order propagators $P_{(k>2)}$. A way of doing this properly will be discussed in Sec. III. It may also be noted here that the standard first-order propagator, $P_{(1)}(x_{n+1},\tau|x_n)$, follows from Eq. (29) if one neglects in $M_1(x_n,\tau)$ and $M_2(x_n,\tau)$ terms of order τ^2.

For completeness we also present the generalization of Eq. (30) to systems with more than one degree of freedom. It reads

$$P_{(2)}(\mathbf{q}^{n+1},\tau|\mathbf{q}^n)=\{(2\pi)^m\det[M_{ij}(\mathbf{q}^n,\tau)]\}^{-1/2}\times\exp\{-\tfrac{1}{2}M^{ij}(\mathbf{q}^n,\tau)[\mathbf{q}_i^{n+1}-M_i(\mathbf{q}^n,\tau)][]_j\}, \tag{32}$$

where

$$M_i=\left[q_i+\tau G_i+\frac{\tau^2}{2}\left(G_j\partial_jG_i+\frac{1}{2}B_{jk}B_{rk}\partial_{jr}^2G_i\right)\right]_{\mathbf{q}^n},$$

$$M_{ij}=\left[\tau B_{ir}B_{jr}+\frac{\tau^2}{2}\left(B_{ir}B_{kr}\partial_kG_j+B_{jr}B_{kr}\partial_kG_i+G_r\partial_rB_{ik}B_{jk}+\frac{1}{2}B_{rk}B_{pk}\partial_{rp}^2B_{iv}B_{jv}\right)\right]_{\mathbf{q}^n}. \tag{33}$$

The propagator corresponding to the Stratonovich interpretation of Eq. (2) is then obtained from the observation that this equation is the same as the Ito stochastic differential equation but with the drift vector G_i replaced by $G_i+\frac{1}{2}B_{kj}\partial_kB_{ij}$ [4].

Finally, we note that the method outlined above can be modified to cover non-Markovian processes with an arbitrary correlation function. These equations occur in many branches of physics and chemistry, but their solution is a far from simple task. We are going to consider this point in a future publication.

III. THE RELATION WITH THE CUMULANT GENERATING FUNCTION FORMALISM

Within the context of the Fokker-Planck description, the starting point for the derivation of a discrete path integral is the fact that the propagator for a finite time t can be factored into a product of N propagators, each one of which propagates the system for a shorter time interval $\tau=t/N$:

$$P(\mathbf{q},t)=\int\prod_{n=0}^{N-1}d\mathbf{q}^nP(\mathbf{q}^{n+1},\tau|\mathbf{q}^n)P(\mathbf{q}^0,0). \tag{34}$$

The only advantage of breaking up the propagator according to Eq. (34), is that we can thus use, in the right-hand side of this equation, instead of the exact propagator $P(\mathbf{q}^{n+1},\tau|\mathbf{q}^n)$ its short time approximation $P_{(k)}(\mathbf{q}^{n+1},\tau|\mathbf{q}^n)$ leading us to Eq. (5). The most common procedure of approximating the propagator by a discrete path integral relies on the operator representation

$$P(\mathbf{q},t|\mathbf{q}^0)=e^{tL}\delta(\mathbf{q}-\mathbf{q}^0),\quad e^{tL}=(e^{\tau L})^N. \tag{35}$$

The Trotter splitting can then be used which is based on partitioning the Fokker-Planck operator L into a linear contribution L_0 and an anharmonic correction L_1, and approximating each short time evolution operator $\exp(\tau L)$ by a product of exponentials [27],

$$\exp(\tau L)=\exp(\tau L_1/2)\exp(\tau L_0)\exp(\tau L_1/2)+O(\tau^3). \tag{36}$$

The disadvantage of this approach is that its utility is generally restricted to $k\leqslant 2$. Although formally possible to construct, any higher-order approximants involve either polynomials of order k of the operators L_0 and L_1 [29] or negative coefficients [30], making these approximants rather impractical for stochastic processes.

An alternative method of approximating the propagator for short time τ can be developed in terms of the characteristic function formalism without the necessity of introducing noncommuting operators into the discussion. The key point of this approach is the observation that the stochastic dynamics can be studied in a formally equivalent way by following either the distribution function or the average of dynamical variables defined by

$$\langle a(t)\rangle=\int d\mathbf{q}\;P(\mathbf{q},t)a(\mathbf{q}). \tag{37}$$

It is a simple matter to show that Eq. (37) can be cast into the form

$$\langle a(t)\rangle = \int d\mathbf{q}\; P(\mathbf{q},0)A(\mathbf{q},t), \tag{38}$$

where the function $A(\mathbf{q},t)$ obeys the backward Fokker-Planck equation

$$\partial_t A(\mathbf{q},t) = L^+ A(\mathbf{q},t) \equiv [G_i(\mathbf{q})\partial_i + \tfrac{1}{2}D_{ij}(\mathbf{q})\partial_{ij}^2]A(\mathbf{q},t), \tag{39}$$

supplemented by the initial condition $A(\mathbf{q},0)=a(\mathbf{q})$. With a δ-function initial condition

$$P(\mathbf{q},0|\mathbf{q}^0) = \delta(\mathbf{q}-\mathbf{q}^0), \tag{40}$$

the formal solution of the above problem reads

$$\langle a(t)\rangle = [\exp(tL^+)a(\mathbf{q})]_{\mathbf{q}^0}. \tag{41}$$

Our aim is to develop a *systematic* strategy for generating short time propagators in terms of the known averages of dynamical variables. A straightforward way for achieving this is to make use of the characteristic function. The latter is defined by

$$\varphi(\mathbf{z}) = \int d\mathbf{q}\; P(\mathbf{q},t)\exp(\imath\mathbf{q}^T\mathbf{z}) \tag{42}$$

and can be evaluated in terms of moments by expanding it as a power series

$$\varphi(\mathbf{z}) = \frac{\imath^r}{r!}\sum_{\{\nu\}}\langle q_1^{\nu_1}\cdots q_m^{\nu_m}\rangle \frac{r!}{\nu_1!\cdots\nu_m!}\,\delta\Big(r,\sum_{j=1}^{m}\nu_j\Big) \times z_1^{\nu_1}\cdots z_m^{\nu_m}, \tag{43}$$

where the index of summation r varies from 1 to ∞. When the moments $\langle\Pi_i q_i^{\nu_i}\rangle$ are all determined, e.g., by Eq. (41), the Fourier inversion formula

$$P(\mathbf{q},t) = (2\pi)^{-m}\int d\mathbf{z}\;\varphi(\mathbf{z})\exp(-\imath\mathbf{q}^T\mathbf{z}) \tag{44}$$

gives us the distribution function $P(\mathbf{q},t)$ for an arbitrary time t. As, however, we are interested in the short time dynamics, a truncated power series representation for the moments,

$$\Big\langle\prod_{i=1}^{m} q_i^{\nu_i}\Big\rangle_{(k)} = \Big[\sum_{j=0}^{k}\frac{(\tau L^+)^j}{j!}\prod_{i=1}^{m} q_i^{\nu_i}\Big]_{\mathbf{q}^n} = \sum_{j=0}^{k} A_j(\mathbf{q}^n)\tau^j,$$

$$(j+1)A_{j+1}(\mathbf{q}^n) = [L^+A_j(\mathbf{q})]_{\mathbf{q}^n}, \quad A_0(\mathbf{q}) = \prod_{i=1}^{m} q_i^{\nu_i} \tag{45}$$

could be used to determine the short time propagator $P_{(k)}(\mathbf{q}^{n+1},\tau|\mathbf{q}^n)$ via Eqs. (43) and (44). The disadvantage of this approach, however, is that the moment expansion, Eq. (43), does not correspond to any systematic expansion in a parameter of the system. As a result, one has to determine and sum infinitely many terms in the series (43) whatever small τ we chose. Otherwise it may diverge even though $\tau=0$.

Fortunately, this is not the case for the cumulant generating function defined by

$$\Phi(\mathbf{z}) = \ln\varphi(\mathbf{z}). \tag{46}$$

It is also expandable in a power series that can be written as

$$\Phi(\mathbf{z}) = \frac{\imath^r}{r!}\sum_{\{\nu\}}\langle\langle q_1^{\nu_1}\cdots q_m^{\nu_m}\rangle\rangle\,\delta\Big(r,\sum_{j=1}^{m}\nu_j\Big)z_1^{\nu_1}\cdots z_m^{\nu_m}, \tag{47}$$

where the quantities $\langle\langle q_1^{\nu_1}\cdots q_m^{\nu_m}\rangle\rangle$ are called the cumulants of the variables $\mathbf{q}$. The notation chosen should not be taken to mean that the cumulants are functions of the particular product of powers of the $\mathbf{q}$. It rather indicates the moment of highest order which occurs in their expression in terms of moments. The cumulants can be evaluated in terms of moments by inserting Eqs. (43) and (47) into Eq. (46), expanding the logarithm in a power series and equating like powers in $\mathbf{z}$. This gives the following expressions for the first few cumulants:

$$\langle\langle q_i\rangle\rangle \equiv M_i = \langle q_i\rangle,$$

$$\langle\langle q_iq_j\rangle\rangle \equiv M_{ij} = \langle q_iq_j\rangle - \langle q_i\rangle\langle q_j\rangle,$$

$$\langle\langle q_iq_jq_k\rangle\rangle \equiv M_{ijk} = \langle q_iq_jq_k\rangle - \langle q_iq_j\rangle\langle q_k\rangle - \langle q_i\rangle\langle q_jq_k\rangle - \langle q_iq_k\rangle\langle q_j\rangle + 2\langle q_i\rangle\langle q_j\rangle\langle q_k\rangle, \tag{48}$$

which are valid for any number of equal i,j,k. An explicit general formula for converting moments into cumulants can be found in Ref. [4].

Although both representations are formally equivalent, the cumulant expansion (47) presents the more natural choice for our purpose. The advantage of this representation is that just the first two cumulants, namely, the means $\langle q_i\rangle$ and covariances $\langle q_i,q_j\rangle$ mainly contribute to Eq. (47) for τ going to zero; while higher-order cumulants contain information of decreasing significance, unlike higher-order moments. This becomes more evident if one considers for a moment a one-dimensional stochastic process with a constant diffusion coefficient. In this case, Eq. (45) gives

$$\langle x^i\rangle = x_n^i + \tau[i(i-1)x_n^{i-2}D + ix_n^{i-1}G_n] + O(\tau^2), \tag{49}$$

from which follows that we cannot set all moments higher than a certain order to zero, since $\langle x^{2i}\rangle \geqslant \langle x^i\rangle^2$ and thus, all moments contain information about lower moments. For cumulants, however, we have

$$\langle\langle x\rangle\rangle = M_1(x_n,\tau) = x_n + O(\tau),$$

$$\langle\langle x^2\rangle\rangle = M_2(x_n,\tau) = \tau D + O(\tau^2),$$

$$\langle\langle x^3\rangle\rangle = M_3(x_n,\tau) = \tau^3 D^2 G_n'' + O(\tau^4),$$

$$\langle\langle x^k\rangle\rangle = M_k(x_n,\tau) = O(\tau^k) \quad (k>3). \tag{50}$$

This means that in constructing the short time propagator $P_{(k)}$ in terms of the cumulant generating function we can consistently set in Eq. (47) $\langle\langle x^{k+1}\rangle\rangle = 0$, i.e.,

$$P_{(k)}(x_{n+1},\tau|x_n)=(2\pi)^{-1}\int_{-\infty}^{\infty}dz\exp\left[-\imath x_{n+1}z+\sum_{r=1}^{k}\frac{\imath^r}{r!}M_r(x_n,\tau)z^r\right],\quad k>1. \quad (51)$$

The cumulants involved in Eq. (51) are to be evaluated to order τ^k, e.g., in terms of Eq. (45). Although another much more accurate power series expansion for moments can be used for the present purpose [26,31], we will not do so here to keep the presentation simple. Recall also that the conventional first-order propagator is obtained by retaining in $P_{(2)}$ terms of order τ.

The generalization of Eq. (51) to multidimensional systems is straightforward

$$P_{(k)}(\mathbf{q}^{n+1},\tau|\mathbf{q}^n)=(2\pi)^{-m}\int d\mathbf{z}\,\exp\left[-\imath z_i q_i^{n+1}+\imath M_i(\mathbf{q}^n,\tau)z_i-\frac{1}{2}M_{ij}(\mathbf{q}^n,\tau)z_iz_j-\frac{\imath}{6}M_{ijr}(\mathbf{q}^n,\tau)z_iz_jz_r-\cdots\right],\quad k>1. \quad (52)$$

If one neglects, in the above equation, cumulants of higher order than 2, one immediately obtains

$$P_{(g)}(\mathbf{q}^{n+1},\tau|\mathbf{q}^n)=\{(2\pi)^m\det[M_{ij}(\mathbf{q}^n,\tau)]\}^{-1/2}\times\exp\{-\tfrac{1}{2}M^{ij}(\mathbf{q}^n,\tau)\times[\mathbf{q}_i^{n+1}-M_i(\mathbf{q}^n,\tau)][]_j\}. \quad (53)$$

The above short time propagator is generally valid to order τ^2 with M_i and M_{ij} given by

$$M_i(\mathbf{q}^n,\tau)=\left[q_i+\tau G_i+\frac{\tau^2}{2}\left(G_j\partial_jG_i+\frac{1}{2}D_{kj}\partial_{kj}^2G_i\right)\right]_{\mathbf{q}^n}+O(\tau^3),$$

$$M_{ij}(\mathbf{q}^n,\tau)=\left[\tau D_{ij}+\frac{\tau^2}{2}\left(D_{ik}\partial_kG_j+D_{jk}\partial_kG_i+G_k\partial_kD_{ij}+\frac{1}{2}D_{rk}\partial_{rk}^2D_{ij}\right)\right]_{\mathbf{q}^n}+O(\tau^3). \quad (54)$$

But what is especially pleasing is that for multidimensional systems the cumulant expansion may converge even better than in one dimension, in the sense that the leading term of M_{ijk} may be of order τ^5 rather than τ^3 as in Eq. (50). In this case, the short time propagator $P_{(k)}$ remains Gaussian for $k\leqslant 4$, and can be evaluated in terms of Eq. (53) if one includes in M_i and M_{ij} terms up to order τ^4. Two physically meaningful systems of such a kind will be considered Sec. IV.

If this is not the case, non-Gaussian corrections are to be taken into account in Eq. (52) to obtain $P_{(k>2)}$. Of course, these more accurate propagators are more difficult to evaluate than, say, Eq. (53), but it should not be so dramatic in practical applications. The integral in Eq. (52) could be evaluated approximately having regard to the smallness of non-Gaussian corrections $-(\imath/6)M_{ijr}z_iz_jz_r-\cdots$. One notes, however, that an approximate evaluation of such a kind spoils the normalization

$$\int d\mathbf{q}^{n+1}P_{(k)}(\mathbf{q}^{n+1},\tau|\mathbf{q}^n)=1, \quad (55)$$

which is automatically preserved in Eq. (52). From this point of view, numerical evaluation of the integral in Eq. (52) seems preferable. It can easily be accomplished if one takes advantage of fast Fourier transforms [32]. The favorable scaling of the fast Fourier transforms, which is almost linear with the total number of grid points, allows one to evaluate $P_{(k)}$ to any desired order in τ with a mild increase of computational efforts.

Before closing this section a few remarks are in order. First we note that Eqs. (53) and (54) exactly coincide with our previous result, given by Eqs. (32) and (33), for $\mathbf{D}(\mathbf{q})=\mathbf{B}(\mathbf{q})\mathbf{B}^T(\mathbf{q})$. This is not surprising if one notices that cumulants of higher order than 1 of the systematic variables $\mathbf{q}$ do not contain the deterministic solution, being thus exactly the same as cumulants of the stochastic portion of $\mathbf{q}(t)$ in the corresponding Langevin description. Next we would like to emphasize the exceptional ease with which this general result, Eqs. (53) and (54), has been obtained. It is in drastic contrast to the power series expansion formalism whose utility seems rather doubtful for general stochastic processes [21]. Noteworthy also is the structure of Eq. (53). The exponent of this short time propagator is a rational function of τ, being thus different from a polynomial representation inherent to the power series expansion formalism [see Eq. (18)]. Finally, we note that the method outlined above can be modified to cover truly nonlinear Fokker-Planck equations whose coefficients exhibit a functional dependence on the distribution function $P(\mathbf{q},t)$ [31]. These equations arise very naturally in many branches of physics and chemistry such as plasma physics, nonlinear optics, and theory of nucleation, but their solution, either analytical or numerical, presents a sufficiently difficult and often impossible task.

IV. APPLICATIONS

The aim of this section is twofold. First, we would like to illustrate the power of the various approximations discussed above for the short time propagator in path integral calculations. To this end, a model system is chosen which is simple enough to enable comparison with exact results obtained by other means. Yet another goal is to show the utility of the cumulant expansion formalism in treating processes with singular diffusion matrices. For this purpose, the idea introduced here is directly applied to two of the most extensively studied models, namely, the so-called Kramers and colored-noise models. The corresponding short time propagators are determined explicitly to order τ^4. Our selection is not exhaustive with respect to methodology, but the essentials of the present technique are thought to be well illustrated by these cases. It may also be noted that the models we are going to discuss are commonly used in studies of superionic

conductors, Josephson tunneling junctions, nonlinear optics, nucleation and escape rate theories [5,33]. The essential features of many of these processes mimic the dynamics of potential barrier crossing, a problem which was first treated in a landmark paper by Kramers [2].

A. Path integral calculations

We first illustrate the use of the propagator, present technique by calculating the propagator of a one-dimensional stochastic process. A benchmark model repeatedly studied by many authors, within this context, is

$$\dot{x}=x-x^3+\sqrt{D}F(t), \tag{56}$$

where the noise $F(t)$ is the same as in Eq. (19). The dynamics is that of an overdamped Brownian particle moving in the symmetric bistable potential $U(x)=x^4/4-x^2/2$ with minima at $x_{\pm}=\pm 1$. The process is governed by the Fokker-Planck equation

$$\partial_t P(x,t|x_0)=\left[\partial_x(x^3-x)+\frac{D}{2}\partial_{xx}^2\right]P(x,t|x_0), \tag{57}$$

for which numerically exact results (i.e., can be made arbitrarily accurate) are easily obtained by a finite-difference method described earlier [7]. As Eq. (56) is nonlinear in x, the process is not Gaussian and, therefore, infinitely many terms are generally to be included in Eq. (51) to accurately evaluate the propagator for arbitrarily large t.

Figure 1 shows the accuracy achieved when employing $P_{(k)}(x,t|x_0)$ as *a single time step propagator* compared to the exact solution for different values of t and for $k=1,2$, and 3. The calculation is performed for $x_0=x_-$ and $D=0.1$. The algorithm we used in evaluating $P_{(k>2)}(x,t|x_0)$ to carry out the fast Fourier transform can be found in Ref. [32]. As expected, the various approximations are not very different from the exact solution when the time increment t is small enough. With increasing t, however, the accuracy of the standard first-order propagator $P_{(1)}$ deteriorates very rapidly, and it becomes inadequate for $t>0.1$. The second-order propagator $P_{(2)}$, though more accurate than $P_{(1)}$, also fails to produce correct results for $t>0.2$. The reason is that its range of validity is generally restricted by the inequality $M_2=Dt[1+t(1-3x_0^2)]\geqslant 0$. The same fortunately is not true for higher-order propagators. A considerable reduction of the error over a broad range of t is seen to be already achieved with just the first non-Gaussian correction taken into account [see $P_{(3)}(x,t|x_0)$].

Next, we apply the various approximations discussed above for the short time propagator to the path integral evaluation of the same conditional probability $P(x,t|x_-)$. The calculation is again performed for $D=0.1$. The integrals in Eq. (5) are evaluated iteratively using the primitive rectangular rule

$$P_i(t+\tau)=P_{ij}(\tau)P_j(t)h;\quad P_i(t)=P(x_i,t);$$

$$P_{ij}(\tau)=P_{(k)}(x_i,\tau|x_j), \tag{58}$$

where a uniformly spaced x lattice of J points is introduced reading

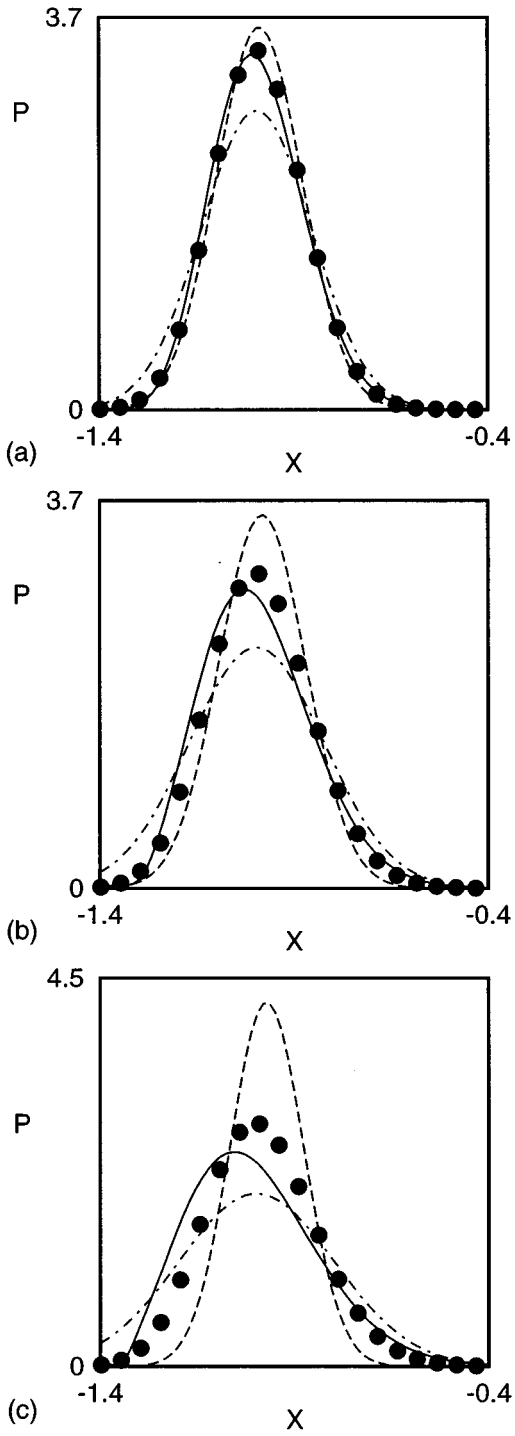

FIG. 1. Probability distribution $P(x,t|x_0)$ for the model (57) for $D=0.1$ and $x_0=-1$. Circles, exact results; dashed lines, first-order propagator; dot-dashed lines, second-order propagator; solid lines, third-order propagator. (a) $t=0.2$, (b) $t=0.3$, and (c) $t=0.4$.

$$x_i=x_1+(i-1)h,\quad i=1,\ldots,J,\quad h=(x_J-x_1)/(J-1).$$

A grid of 64 points in the interval $[-1.6,1.6]$ was found to be sufficient for the quadrature. One might expect that for fixed t and N this discretization procedure would produce, with increasing k, much more accurate results than obtained with the conventional first-order propagator. We have found, however, that the use of the matrix P_{ij} defined by Eq. (58),

regardless of the number k, leads to a trivial long-time limit solution, $P(x,t\to\infty|x_0)=0$, instead of the exact one

$$P_0(x)=\left\{\int_{-\infty}^{\infty}dx\ \exp[-2U(x)/D]\right\}^{-1}\exp[-2U(x)/D]. \tag{59}$$

This is because the matrix P_{ij} does not preserve the norm of the distribution function

$$\sum_{i=1}^{J}P_i(t)h=1 \tag{60}$$

or, equivalently, satisfy the condition

$$\sum_{i=1}^{J}P_{ij}(\tau)h=1 \quad \forall j,\tau. \tag{61}$$

We have found that a dramatic reduction of the discretization error is achieved by a simple procedure of renormalizing the transition matrix elements so that the norm is conserved. Specifically, we enforce Eq. (61) by the following modification of P_{ij}:

$$\tilde{P}_{ij}=\left\{\sum_{k=1}^{J}P_{kj}h\right\}^{-1}P_{ij}. \tag{62}$$

The relative efficacy of different $P_{(k)}$ is demonstrated by calculating the second cumulant $M_2(x_-,t)$ and the matrix element $P(x_-,t|x_+)$. The former characterizes the width of the probability distribution. While the latter is closely related to the first nonzero eigenvalue of the Fokker-Planck operator, λ_1, whose inverse is the largest relaxation time in a double well. For $D=0.1$ the numerically exact result is $\lambda_1=0.002\ 776\ 140\ 8$. Figure 2 shows the relative error

$$\varepsilon=(\text{approximate}-\text{exact})/\text{exact}, \tag{63}$$

in the path integral evaluation of $M_2(x_-,t)$ and $P(x_-,t|x_+)$ made by using $P_{(k)}$ with $k=1$, 2, and 3 as a function of t. The calculation is performed with fixed $\tau=0.1$. As evidenced by Fig. 2, the error, being usually maximal at $t=\tau$, reaches zero for $\lambda_1 t\sim 2.5$ and then slowly increases with t going to infinity until a stationary value is achieved. It is also seen that the error made by the standard first-order propagator $P_{(1)}$ is large compared to that of the cumulant expansion. Although no non-Gaussian correction appears in $P_{(2)}$ in the present treatment, the effect of retaining terms of order τ^2 is the reduction of the error roughly by a factor of 4. The non-Gaussian third-order propagator is seen to further reduce the error again by a factor of 4. The treatment is fairly straightforward and can be carried out systematically until a given level of accuracy is reached. Next, we present in Fig. 3 results obtained with $P_{(3)}$ for different values of τ. A comparison of Figs. 2 and 3 shows that the errors made by using $P_{(2)}$ and $P_{(1)}$ with $\tau=0.1$ are almost the same as those of $P_{(3)}$ obtained with $\tau=0.2$ and 0.3, respectively. This means that results to a given level of accuracy are obtained with a smaller value of N. Finally, we illustrate the efficacy of the present technique in giving precise long-time limit results. The exact stationary solution,

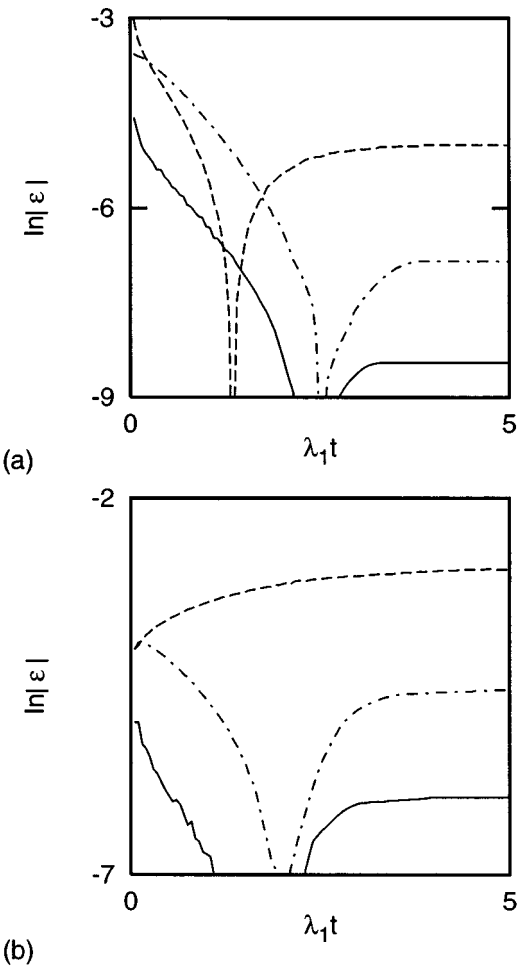

FIG. 2. Logarithm of the relative error $\ln|\varepsilon|$ [Eq. (63)] in the path integral evaluation, with $\tau=0.1$, of (a) the second cumulant $M_2(x_-,t)$, and (b) the matrix element $P(x_+,t|x_-)$ for the model (57) for $D=0.1$ and $x_\pm=\pm 1$. The dashed, dot-dashed, and solid lines are, respectively, for the results obtained using $P_{(k)}$ with $k=1$, 2, and 3. In the abscissa, λ_1 is the first nonzero eigenvalue of the Fokker-Planck operator.

Eq. (59), is shown in Fig. 4 and compared with that obtained by using $P_{(1)}$ and $P_{(3)}$ with $\tau=0.2$, and 0.4 for $\lambda_1 t=10$. It is seen that an adequate description is achieved even though $\tau=0.4$. This is in drastic contrast to the finite-difference schemes currently used to solve Fokker-Planck equations numerically. These schemes do not provide automatically the positivity of the solution, thus restricting the size of the time increment τ and requiring very fine time slicing. With increasing τ they very rapidly become unstable and may fail grossly.

Before closing we note that the accuracy of an iterative path integral method is typically determined by the accuracy of the space and time discretizations. The standard way to control it is thus by increasing the number of grid points J and time slices N. In practice, however, one would like these numbers to be as small as possible, in order to achieve computational economy. The accuracy of the space discretization can be substantially improved if one uses, instead of the primitive histogram representation of the probability distribution, a more accurate quadrature scheme. While taking advantage of the present technique allows one to achieve a

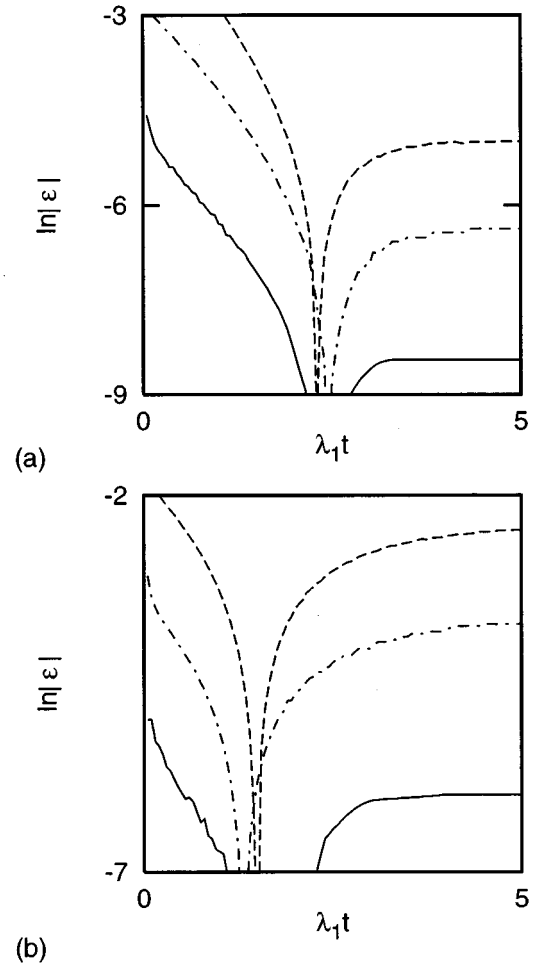

FIG. 3. Same as in Fig. 2, but for the third-order propagator. The solid, dot-dashed, and dotted lines are for $\tau=0.1$, 0.2, and 0.3, respectively.

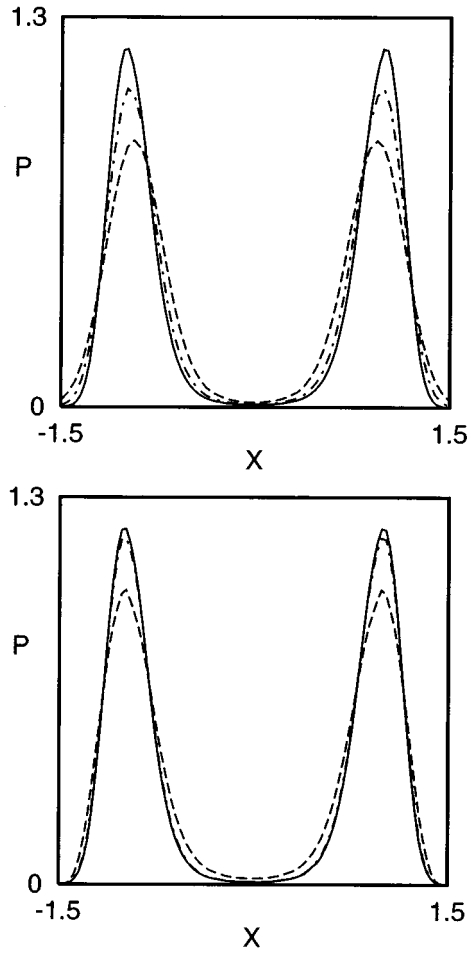

FIG. 4. Stationary distribution for the model (57) for $D=0.1$. The solid line is the exact result, Eq. (59). The dot-dashed and dashed lines show, respectively, the path integral evaluation with $\tau=0.2$ and 0.4. (a) First-order propagator, and (b) third-order propagator.

given level of accuracy with a slow (or even without) increase of the number of time steps solely due to increasing k.

B. Kramers model

The Kramers model is described by two coupled Langevin equations which read in dimensionless variables

$$\dot{x}=v, \quad \dot{v}+\gamma v-G(x)=\sqrt{2\gamma\varepsilon}F(t), \tag{64}$$

with $F(t)$ being Gaussian white noise defined by Eq. (20). In the above γ is the friction coefficient, and ε is a measure of the noise intensity. The dynamics described by the model is that of a Brownian particle moving in a potential

$$U(x)=-\int^{x} dy G(y). \tag{65}$$

This process is governed by the following Fokker-Planck equation (also called the Klein-Kramers equation) for the probability density of finding the particle at time t at position x with velocity v

$$\partial_t P(x,v,t)=[-v\partial_x-G(x)\partial_v+\gamma\partial_v(v+\varepsilon\partial_v)]P(x,v,t). \tag{66}$$

It is not hard to see that the diffusion matrix of Eq. (66) does not possess an inverse.

The continuous time path integral solution for the above process is easily obtained by using Eq. (64) to transform the probability density functional for the noise, which is given by

$$P[F(t)]=C\ \exp\left[-\frac{1}{4\gamma\varepsilon}\int_0^t ds F^2(s)\right], \tag{67}$$

with C being a normalization constant, to the probability density functional for the coordinate x

$$P[x(t)]=CJ[x(t)]\exp\left\{-\frac{1}{4\gamma\varepsilon}\int_0^t ds[\ddot{x}+\gamma\dot{x}-G(x)]^2\right\}, \tag{68}$$

where $J[x(t)]$ denotes the Jacobian of the transformation from the $F(t)$ realizations to the $x(t)$ realizations. One sees, however, that this solution is purely formal and, therefore, no

simpler to implement numerically than the original Fokker-Planck or Langevin equations.

By contrast, the formalism developed here offers a convenient tool for the systematic treatment of the Kramers problem both analytically and numerically. Keeping terms up to $O(\tau^4)$ in Eq. (45), one obtains that the first cumulants of the variables (x,v) are given by the expressions

$$M_x = x_n + \tau v_n + \frac{\tau^2}{2}(G_n - \gamma v_n) + \frac{\tau^3}{6}[\gamma^2 v_n - \gamma G_n + v_n G_n'] + \frac{\tau^4}{24}[\gamma^2 G_n - \gamma^3 v_n + G_n'(G_n - 2\gamma v_n) + v_n^2 G_n''],$$

$$M_v = v_n + \tau(G_n - \gamma v_n) + \frac{\tau^2}{2}[\gamma^2 v_n - \gamma G_n + v_n G_n'] + \frac{\tau^3}{6}[\gamma^2 G_n - \gamma^3 v_n + G_n'(G_n - 2\gamma v_n) + v_n^2 G_n''] + \frac{\tau^4}{24}[\gamma^4 v_n - \gamma^3 G_n + G_n'(3\gamma^2 v_n - 2\gamma G_n + v_n G_n') + G_n''(2\gamma\varepsilon + 3 v_n G_n - 4\gamma v_n^2) + v_n^3 G_n'''],$$

$$M_{xx} = \tfrac{2}{3}\gamma\varepsilon\tau^3(1 - \tfrac{3}{4}\gamma\tau),$$

$$M_{xv} = \gamma\varepsilon\tau^2[1 - \gamma\tau + \tfrac{1}{12}\tau^2(7\gamma^2 + 4G_n')],$$

$$M_{vv} = 2\gamma\varepsilon\tau[1 - \gamma\tau + \tfrac{1}{3}\tau^2(2\gamma^2 + G_n') - \tfrac{1}{12}\tau^3(4\gamma^3 + 5\gamma G_n' - 3 v_n G_n'')], \quad (69)$$

while all cumulants of higher order than 2 vanish. The latter property implies that the Gaussian approximation for the short time propagator, Eq. (53), remains correct up to and including terms of order τ^4. This immediately yields

$$P_{(4)}(x_{n+1}, v_{n+1}, \tau | x_n, v_n) = (4\pi^2 M)^{-1/2} \exp\left[-\frac{M_{vv}}{2M}(x_{n+1} - M_x)^2 + \frac{M_{xv}}{M}(x_{n+1} - M_x)(v_{n+1} - M_v) - \frac{M_{xx}}{2M}(v_{n+1} - M_v)^2 \right], \quad (70)$$

where $M = M_{xx}M_{vv} - M_{xv}^2$. Recall that the cumulants M_x, M_v, M_{xx}, M_{xv}, M_{vv} involved in Eq. (70) are functions of τ and of the prepoint (x_n, v_n) [see Eq. (69)], but to keep the notation simple we do not indicate this explicitly.

As evidenced by Eq. (69), the range of validity of the above single step propagator is rather sensitive to the friction coefficient. The time increment τ should always be taken small enough in the high friction limit $\gamma \to \infty$ so that to keep the integration measure positive, and may be taken large enough otherwise. We also emphasize that its utility is restricted to $3 \leqslant k \leqslant 4$. For lower k the matrix element M_{xx} becomes equal to zero and the singularity problem is met in this case. While for $k \geqslant 5$, higher-order cumulants of the variables (x,v) are no longer equal to zero and non-Gaussian corrections are needed. Substitution of Eq. (70) into Eq. (5) yields the discrete path integral representation of the Kramers problem we are looking for. This representation is as powerful in formal manipulations as the continuous time integral solution, Eq. (68), and still permits one to devise very efficient algorithms for numerical simulations which cannot be developed in terms of partial [Eq. (66)] or stochastic [Eq. (64)] differential equations.

C. Colored-noise problem

Another example is a process subjected to external noise with a finite correlation time, so-called colored noise. It is governed by a one-dimensional non-Markovian Langevin equation of the form

$$\dot{x} = G(x) + v(t), \quad (71)$$

where the fluctuating force $v(t)$ is assumed to be a nonwhite Gaussian process with statistical properties

$$\langle v(t) \rangle = 0, \quad \langle v(t) v(s) \rangle = \varepsilon\sigma(t - s). \quad (72)$$

An important situation repeatedly studied by many authors is the case of $v(t)$ being an Ornstein-Uhlenbeck process, i.e.,

$$\dot{v} = \gamma[-v + \sqrt{2\varepsilon}F(t)], \quad (73)$$

with γ^{-1} being the correlation time of the noise. The white noise term $F(t)$ and the quantity ε appearing in the above equations are exactly the same as in Eq. (64). Since $F(t)$ is Gaussian and has a zero mean, the noise $v(t)$ is also Gaussian with the correlation function

$$\langle v(t) v(s) \rangle = \varepsilon\gamma \exp(-\gamma|t - s|). \quad (74)$$

When γ goes to infinity (short correlation times), one can completely neglect the term $\dot{v}$ in Eq. (73), thus reducing the problem to that already studied in the previous sections. For finite γ's the Fokker-Planck equation describing the pair stochastic process $(x(t), v(t))$ reads

$$\partial_t P(x,v,t) = \{-\partial_x[G(x) + v] + \gamma\partial_v(v + \varepsilon\gamma\partial_v)\} P(x,v,t). \quad (75)$$

As is the case with Eq. (66), the diffusion matrix of the above equation is singular. Moreover, the Fokker-Planck dynamics for the pair $(x(t), v(t))$ does not obey detailed balance.

Following the line outlined in the preceding section, it is not hard to show that the short time propagator valid to order τ^4 for the above process has the same form as in Eq. (70), but cumulants are now given by

$$M_x = x_n + \tau(G_n + v_n) + \frac{\tau^2}{2}[(G_n + v_n)G_n' - \gamma v_n] + \frac{\tau^3}{6}[v_n(\gamma^2 - \gamma G_n') + (G_n + v_n)G_n'^2 + (G_n + v_n)^2 G_n''] + \frac{\tau^4}{24}[(G_n + v_n)(G_n'^3 - 3\gamma v_n G_n'') - \gamma v_n(G_n'^2 + \gamma^2$$

$$-\gamma G_n')+2\varepsilon\gamma^2 G_n''+4(G_n+v_n)^2 G_n' G_n''$$
$$+(G_n+v_n)^3 G_n'''],$$
$$M_v=v_n(1-\gamma\tau+\tfrac{1}{2}\gamma^2\tau^2-\tfrac{1}{6}\gamma^3\tau^3+\tfrac{1}{24}\gamma^4\tau^4),$$
$$M_{xx}=\tfrac{2}{3}\varepsilon\gamma^2\tau^3[1+\tfrac{3}{4}\tau(G_n'-\gamma)],$$
$$M_{vv}=2\varepsilon\gamma^2\tau(1-\gamma\tau+\tfrac{2}{3}\gamma^2\tau^2-\tfrac{1}{3}\gamma^3\tau^3),$$
$$M_{xv}=\varepsilon\gamma^2\tau^2\left[1+\frac{\tau}{3}(G_n'-3\gamma)+\frac{\tau^2}{12}(7\gamma^2-4\gamma G_n'+G_n'^2\right.$$
$$\left.+3G_nG_n''+3v_nG_n'')\right]. \quad (76)$$

It may be noted here that the remarks made below Eq. (70) are all valid in this case as well. Finally, we would like to emphasize that aside from the two aforementioned models that are currently investigated by the present author, this formalism can also be applied to many other fields involving Fokker-Planck and Langevin equations.

V. CONCLUSIONS

In this work, the cumulant expansion formalism is presented which permits one to generate a high-accuracy discrete path integral representation of stochastic dynamics. The method is rather simple to implement, but also general and rigorous and allows for the *systematic* derivation of the short time propagator valid to any desired precision in time increment τ. Another attractive feature of the present technique when compared to the others known in the literature, is that it is applicable, whether the diffusion matrix is invertible or singular. Numerical applications to the conditional probability in a double well shows this approach to be a dramatic improvement over the standard first-order propagator. Its use in a path integral means a significant reduction of the number of time steps that are required to achieve a given level of accuracy and, therefore, significantly increasing the feasibility of path integral calculations. In view of this it is difficult to overstate the usefulness of the path integral formulation in treating numerically multidimensional systems. This will be the subject of our future publications, but let us briefly mention here the methods available.

Two general approaches are possible: one can integrate Eq. (5) iteratively or use global integration (Monte Carlo) techniques. Each approach has its own advantages and drawbacks. In studying one-, two-, or three-dimensional systems, when storage requirements are not so dramatic yet, the iterative evaluation of the mN integral in Eq. (5) is preferable. Efforts along this line has been quite successful, and a number of iterative schemes have been developed that are computationally efficient in terms of speed [20]. High proficiency is achieved by using fast Fourier transforms [34]. The latter becomes particularly important if mN is large, as is the case when a few coupled degrees of freedom are involved and/or simulations over very long times are required. If the number of coupled degrees of freedom is too large, the mN integral in Eq. (16) must be evaluated by Monte Carlo techniques [35]. The most appealing feature of this approach is that it avoids storing large dimensional matrices. Instead, the mN integral in Eq. (5) is evaluated by moving repeatedly from point to point on the space-time lattice, at each point proposing a change in the coordinates, and accepting the change via the Metropolis algorithm [35]. The use of this procedure allows for the efficient treatment of truly multidimensional systems without introducing uncontrolled approximations. Moreover, it is often the case that computational effort necessary for obtaining the numerically exact solution grows slowly with substantial dimensionality increases due to importance Monte Carlo sampling techniques [35].

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