Accurate path integral representations of the Fokker-Planck equation with a linear reference system: Comparative study of current theories

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This paper presents an application of new discrete path integral solutions recently introduced for Fokker-Planck dynamics with the aim to compare their relative efficacy in giving precise numerical results. The basic idea used in the derivation of these solutions is to model a complex Fokker-Planck equation with a general drift coefficient by a linear (Ornstein-Uhlenbeck) process, which is solved exactly, and to then employ an iterative technique to quantify what is missing from the reference description. We reexamine and analyze two different approaches to realize the above strategy. These are an operator decoupling technique and a power series expansion method. Both approaches allow one to construct higher-order propagators valid to any desired precision in a time increment τ. Their use in a path integral means that *many* fewer time steps N are required to achieve a given accuracy for a given net increment $t = N\tau$. Our comparison also includes results from standard path integral representations. The relative efficacy of the various different methods is illustrated by means of two problems, namely, the dynamics of an overdamped Brownian particle in a potential field and the Kramers model of chemical reaction. The former process can be modeled by a one-dimensional Fokker-Planck equation for the position coordinate only, while the latter is governed by a two-dimensional Fokker-Planck equation where the relaxation over velocity is taken into account. The numerical applications clearly demonstrate that the new representations are superior in the sense that they yield much more *accurate* results with *less* computational effort than the best alternative path integral method now in use. [S1063-651X(98)02001-7]

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I. INTRODUCTION

There is a wide variety of phenomena in physics, chemistry, and biology whose dynamics is accurately described in terms of a Fokker-Planck equation. It is a mesoscopic kinetic equation for the distribution function $P(\mathbf{q},t)$ involving a deterministic drift vector $\mathbf{G}$ and a diffusion tensor $\mathbf{D}$. The former describes the deterministic path of the system, while the latter incorporates fluctuations away from this path. The equation typically has the form

$$\partial_t P(\mathbf{q},t) = LP(\mathbf{q},t) \equiv [-\partial_i G_i(\mathbf{q}) + \tfrac{1}{2} D_{ij} \partial_{ij}^2] P(\mathbf{q},t), \tag{1.1}$$

where the standard summation convention over repeated indexes is implied, $\mathbf{q} = \{q_1, \ldots, q_n\}$, and L is the Fokker-Planck operator defined by Eq. (1.1). In the study of time evolution of the processes governed by Eq. (1.1) much information can be found from the investigation of the propagator, which is the fundamental solution of the equation satisfying the initial condition

$$P(\mathbf{q},0|\mathbf{q}^0) = \delta(\mathbf{q} - \mathbf{q}^0). \tag{1.2}$$

Specific examples of Fokker-Planck equations can be drawn from a vast amount of different fields ranging from nuclear physics to communication theory [1,2]. The flexibility of the above description makes Eq. (1.1) very attractive both for theoreticians and for experimentalists. From an experimental

point of view, an appealing feature of the Fokker-Planck equation is that it provides a very useful statistical model for understanding various dynamical processes in realistic systems driven by noise and friction. Some theoretical aspects of the Fokker-Planck equation are still under intensive study. Many challenges have a single origin: analytical solutions to the Fokker-Planck equation are available for a few simple cases, and virtually all nontrivial problems cannot be solved exactly with presently known mathematical techniques. This situation has led to the search for approximate methods to analyze such problems either analytically or numerically. All these methods are efficient in treating one-dimensional problems. Some of them remain efficient in two dimensions, and just a few methods can be applied to systems with more than two degrees of freedom.

In this context, it is difficult to overemphasize the usefulness of the path integral approach to Fokker-Planck dynamics. Being formally exact, it provides a global solution (integral formulation) of the problem in question, which is, in principle, amenable to approximations. Several approximate schemes could be efficient in analytically treating this solution in arbitrary dimensions, provided that the specific assumptions on which they are based are satisfied. Numerical applications have also increased enormously over the past decade, yielding important new insights into the behavior of complex physical systems. From a computational point of view, one of the great advantages of the path integral formulation is that it reduces the problem of solving the Fokker-Planck equation to the evaluation of an integral whose dimension grows *linearly* with the number of coupled degrees of freedom. The starting point for its derivation is the fact that the propagator for a finite time t can be factored into a product of N propagators, each of them describing the evo-

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lution of the system for a shorter time interval $\tau = t/N$,

$$P(\mathbf{q}, t | \mathbf{q}^0)$$

$$= \int d\mathbf{q}^{N-1} \cdots \int d\mathbf{q}^1 P(\mathbf{q}, \tau | \mathbf{q}^{N-1}) \cdots P(\mathbf{q}^1, \tau | \mathbf{q}^0). \tag{1.3}$$

Clearly, the above equation is exact for any number of time slices N. The only thing that requires N to be large is that the approximation used for the short time, or single step propagator in the right-hand side of Eq. (1.3),

$$P(\mathbf{q}^{i+1}, \tau | \mathbf{q}^i) = P_{(k)}(\mathbf{q}^{i+1}, \tau | \mathbf{q}^i) + O(\tau^{k+1}), \tag{1.4}$$

be sufficiently accurate. Hereby, k is the order of approximation. With the replacement given by Eq. (1.4), the problem is reduced to the calculation of a multidimensional integral (also referred to as a discrete path integral)

$$P(\mathbf{q}, t | \mathbf{q}^0) = \int d\mathbf{q}^{N-1} \cdots \int d\mathbf{q}^1 P_{(k)}(\mathbf{q}, \tau | \mathbf{q}^{N-1}) \cdots P_{(k)}$$
$$\times (\mathbf{q}^1, \tau | \mathbf{q}^0) + O(t^{k+1}/N^k). \tag{1.5}$$

This equation expresses the distribution function for an arbitrary time t in terms of the known short time propagator. As there exists no unique way to determine the short time propagator, many different path integral representations corresponding to various different approximate schemes have resulted [3] (for a recent review see also Ref. [4]). In the continuous time limit $N \to \infty, \tau \to 0$, these representations become exact, but they are, in general, unsolvable. Both continuous and discrete path integral representations are relevant. The former yield a new conceptual basis for understanding the physics described by the Fokker-Planck equation, and the latter provide a powerful tool for obtaining detailed numerical solutions that can be made arbitrarily accurate. Unlike other methods, the path integral solution remains stable for rather large time steps τ and permits the efficient treatment of multidimensional systems without introducing uncontrolled approximations. This is achievable by taking advantage of Monte Carlo techniques, which avoid explicit reference to distribution functions and thus circumvent storing large dimensional matrices. In studying low dimensional systems, when storage requirements are not so dramatic yet, the iterative evaluation of Eq. (1.5) is preferable. It yields numerical results free of statistical errors.

The practical applicability of the numerical schemes available for both global and iterative evaluation of the discrete path integral depends critically on the dimension of the latter. Therefore, higher-order short time propagators, accurate for as long a time τ as possible, are generally desirable. The obvious reason for this is that the higher the rate of convergence of a path integral, the smaller the number of integration variables (and therefore the execution time) that are required to evaluate it to a given accuracy. Until recently, however, the only requirement usually made on the short time propagator was that it satisfies Eq. (1.1) to order $O(\tau)$. For example, one of the commonly used path integral representations is based on the primitive first-order propagator reading

$$P_{(1)}(\mathbf{q}, \tau | \mathbf{q}^0) = [(2\pi\tau)^m \det\mathbf{D}]^{-1/2} \exp\left\{ -\frac{1}{2\tau} [\mathbf{q} - \mathbf{q}^0 \right.$$
$$\left. - \tau\mathbf{G}(\mathbf{q}^0)] \cdot \mathbf{D}^{-1} [\mathbf{q} - \mathbf{q}^0 - \tau\mathbf{G}(\mathbf{q}^0)] \right\}. \tag{1.6}$$

It is obtained by replacing in Eq. (1.1) the true drift vector $\mathbf{G}(\mathbf{q})$ by a constant vector $\mathbf{G}(\mathbf{q}^0)$ or, in other words, by mapping the solution of a difficult problem onto a simpler "zero-order" free-particle reference system, which is solved exactly. This derivation reflects the fact that only the first two cumulants, namely, the means

$$\langle \mathbf{q} \rangle = \mathbf{q}^0 + \tau\mathbf{G}(\mathbf{q}^0) + O(\tau^2) \tag{1.7}$$

and the covariances

$$\langle\langle q_i q_j \rangle\rangle = \tau D_{ij} + O(\tau^2) \tag{1.8}$$

contribute to the Fokker-Planck equation to order $O(\tau)$, while higher-order cumulants (as well as higher-order terms) contain information of decreasing significance and, therefore, can be neglected in the limit $\tau \to 0$. However, the error made by using the primitive propagator (1.6) is of order $1/N$ and thus very short time steps are necessary for accuracy [5]. Accordingly, the dimension of the resulting integral, Eq. (1.5), can be very high if the required propagation time is long [6].

The above observations have inspired the search for more efficient short time propagators, which would provide a given precision with a smaller value of N. A great deal of work has been recently devoted to resolving this problem, and a number of new theoretical approaches have been developed [7–9]. The most appealing feature of these approaches is perhaps that they allow one to *systematically* construct path integral representations of Fokker-Planck dynamics valid to *any* desired order in $1/N$. It is our purpose here to demonstrate the computational utility of the higher-order representations in concrete realistic models, and compare it with the efficacy of standard path integral methods now in use. Finally, to conclude this introduction we note that there are many impressive reviews on path integrations in quantum statistics and mechanics [10]. However, the same analysis of path integral methods for stochastic processes was rare up to recent times.

The remainder of the paper is organized as follows. In Sec. II two higher-order path integral methods are outlined with some improvements and their limitations are discussed. Numerical examples illustrating the power of various different path integral techniques are presented in Sec. III. They include the dynamics of Brownian motion in a single well potential and in a double well. Section IV ends the paper with final remarks. In order to make our article self-contained, a brief description of the standard methods used for comparison is given in the Appendix.

II. HIGHER-ORDER PROPAGATORS WITH A LINEAR REFERENCE SYSTEM

For notational simplicity, we consider a one-dimensional Fokker-Planck equation

$$\partial_t P(x,t) = LP(x,t) \equiv [-\partial_x G(x) + (D/2)\partial_{xx}^2]P(x,t),$$
(2.1)

which describes the motion of an overdamped Brownian particle in a potential field

$$U(x) = -\int^x dy\, G(y).$$
(2.2)

The drift coefficient $G(x)$ is assumed to be such that the Fokker-Planck operator L is bounded on a finite-dimensional Hilbert space. Moreover, we restrict the discussion to the case of ''natural'' or ''inaccessible'' boundaries [2]. From a mathematical point of view, diffusion problems of such a type are easier to solve since no *external* boundary conditions are required for the determination of the short time propagator. Then, the corresponding equilibrium distribution function reads

$$P_e(x) \equiv P(x,t\to\infty) = Z^{-1}\exp[-2U(x)/D],$$
(2.3)

with Z being a normalization constant. In fact, actual use of the methods described below is not more complicated in many dimensions because high dimensionality does not present special conceptual problems. We also point out that the diffusion coefficient D need not be constant and can be a function of x as well. Besides, with minor modifications to what appears below the Fokker-Planck operator can be time dependent and even exhibit an explicit dependence on the distribution function.

A. Operator decoupling technique

The most common procedure of approximating the propagator by a discrete path integral relies on the operator representation

$$P(x,t|x_0) = e^{tL}\delta(x - x_0),$$
(2.4)

which allows one to rewrite Eq. (1.3) as

$$e^{tL} = (e^{\tau L})^N.$$
(2.5)

Since L is a sum of noncommuting operators, an operator decoupling technique must be used to approximate the exponential operator $\exp(\tau L)$ for short time τ by a product of functions involving each of these operators

$$e^{\tau L} = Q_{(k)}(\tau) + O(\tau^{k+1}),$$

$$Q_{(k)}(\tau)^N = e^{tL} + O(t^{k+1}/N^k).$$
(2.6)

A simple way to achieve this is to divide the Fokker-Planck operator into two parts, $L = A + B$, and employ the symmetric Trotter splitting

$$Q_{(2)}(\tau) = e^{\tau A/2}e^{\tau B}e^{\tau A/2}.$$
(2.7)

The advantage of this breakup is that it is time reversible. The approximate propagator so constructed satisfies the condition

$$Q_{(k)}(-t)Q_{(k)}(t) = 1,$$
(2.8)

as does the exact propagator, $\exp(tL)$. Acting by Eq. (2.7) on a delta function, we arrive at a second-order approximation for the short time propagator whose explicit form depends on partitioning the original Fokker-Planck operator $L = A + B$. A small sample of that work can be found in Ref. [7]. Except for some rigorous inequalities [11], little is known about the nature of the Trotter product formula, Eqs. (2.6) and (2.7). Its convergence as a function of N must be studied for each particular case [12]. However, the neglect of the commutator between A and B is often quite severe, and thus use of the Trotter approximation requires rather fine discretization (i.e., large N) of the path integral.

Until recently, two general approaches were used to overcome the above problem. Various higher-order decompositions were constructed either by explicitly including composite operators of the form $[A,[A,B]]$ into the factorized product [13,14] or by using recursive properties of the Trotter splitting, Eq. (2.7), in order to exclude commutators from considerations [15]. Each approach has its own advantages and drawbacks. Although there has been some recent success in path integral calculations with a composite operator factorization [14], the utility of this approach is generally restricted to a certain class of Fokker-Planck equations for which evaluating the composite operators involved in the factorized product is not a major problem. Otherwise these commutators complicate the expression in such a way that the calculation of the single step propagator may be out of the question even for simple one-dimensional systems. In contrast, multisplit operator factorizations with no commutators are readily determined from the recurrence [15]

$$Q_{(2k)}(\tau) = Q_{(2k-2)}(c_k\tau)Q_{(2k-2)}[(1-2c_k)\tau]Q_{(2k-2)}(c_k\tau),$$
(2.9)

where the coefficients are defined by $2c_k^{2k-1} + (1-2c_k)^{2k-1} = 0$ with $k > 1$. The recursive derivation of $Q_{(2k)}$ starts with the Trotter splitting $Q_{(2)}$, Eq. (2.7), and can be carried out to arbitrarily high orders. The resulting factorization can then be written in the explicit form

$$Q_{(2k)}(\tau) = \prod_i e^{a_i\tau A}e^{b_i\tau B},$$
(2.10)

with coefficients (a_i, b_i) determined by the required order of accuracy. However, there has been no attempt to apply this approach to Fokker-Planck processes. The reason is that, beyond second order, any finite-order factorization of the form (2.10) must produce some negative coefficients a_i and b_i. When applied to the Fokker-Planck equation, this means that negative times appear at some diffusion operators, making these approximants of no practical relevance for stochastic processes.

Here we employ an alternative method to construct higher-order approximations, which has been put forward in Refs. [16,17]. The method combines the principal advantages of the above two approaches, being free of their drawbacks. Its basic idea is to exploit the error structure of Eq. (2.7) to remove time slices errors in Trotter-approximated propagators. An attractive feature of the symmetric Trotter splitting is that an approximate propagator constructed of N products, each of which satisfies Eq. (2.8), has an asymptotic

error expansion in *even* powers of $1/N$ [18]. In such a case, standard extrapolation methods can be applied to Eq. (2.6) to successively eliminate the low-order errors resulting from time discretization. In particular, a Romberg-type approximation for the time evolution operator without the $1/N^2$ error is

$$Q_{(4)}(t) = \tfrac{1}{3}[4Q_{(2)}(t/2N)^{2N} - Q_{(2)}(t/N)^N]. \quad (2.11)$$

The process can always be continued to remove all terms in the error series up to but not including $O(1/N^{2k})$. Although this technique (also referred to as Richardson's deferred approach to the limit) has been known for some time [19], its effective application to path integrals has been fully realized only recently. Schmidt and Lee [16] developed a method for calculating finite temperature properties of quantum systems, which involves the successive evaluation of the density matrix by a Trotter product formula of the form $\exp(-\beta\mathcal{H}) \approx Q_{(2)}(\beta/N)^N$. The calculation is performed for $N = 2,4,6,8,12,16,\ldots$. A polynomial extrapolation is then used to fit the result to a low-order polynomial in $1/N^2$ and to predict the exact density matrix corresponding to infinitely fine substeps. However, the utility of the above procedure is restricted to one-dimensional systems. Only in that case is it possible to generate and store a large number of successive approximations to the true propagator, whereas the efficient treatment with this technique of multidimensional dynamical processes is obviously beyond the computational powers of even the fastest computers.

An alternative procedure that allows one to overcome this problem has been suggested in Ref. [17]. Its key idea is to apply Richardson's extrapolation to the average of dynamical variables

$$\langle g(\mathbf{q})[t]\rangle = \int d\mathbf{q}\, g(\mathbf{q})P(\mathbf{q},t), \quad (2.12)$$

rather than to the propagator itself. The time evolution of $\langle g(\mathbf{q})[t]\rangle$ is represented by a scalar function of one variable for arbitrary dimension of the system. Therefore, no problems of storing and treating large dimensional matrices arise in this case. Starting with some N not necessarily large, one can perform the calculation for several different values N_k, so that each time the number of points is doubled, $N_k = 2^k N$, while the error is reduced by a factor of N^2. The latter is achieved by making use of the combination

$$Q_{(2k+2)}(t) = (2^{2k}-1)^{-1}[2^{2k}Q_{(2k)}(t/2N)^{2N} - Q_{(2k)}(t/N)^N], \quad (2.13)$$

which is a straightforward extension of Eq. (2.11) to arbitrary k. The procedure is carried out until a prescribed error tolerance is met.

The symmetric Trotter splitting we employ here is the same as in earlier works [7,17]. It is based on partitioning the Fokker-Planck operator L into a linear contribution,

$$B = r\partial_x x + (D/2)\partial_{xx}^2, \quad (2.14)$$

with the as yet unknown factor r, which is assumed to be independent of x, and an anharmonic correction,

$$A = -\partial_x \widetilde{G}(x), \quad \widetilde{G}(x) = G(x) + rx. \quad (2.15)$$

The second-order short time propagator is then obtained in terms of Eq. (2.7) to yield [7]

$$P_{(2)}(x,\tau|x_0) = J(x,\tau/2)P_r[H(x,\tau/2),\tau|H(x_0,-\tau/2)]. \quad (2.16)$$

Hereby, $P_r(x,t|x_0)$ is the propagator of the reference Ornstein-Uhlenbeck process, Eq. (2.14),

$$P_r(x,t|x_0) = [2\pi\sigma(t)]^{-1/2}\exp[-(x-e^{-rt}x_0)^2/2\sigma(t)], \quad (2.17)$$

with the variance given by

$$\sigma(t) = D(1-e^{-2rt})/2r, \quad (2.18)$$

$H(x,t)$ is a solution of a deterministic equation of motion

$$\dot{x}(t) = \widetilde{G}[x(t)], \quad x(0) = H, \quad (2.19)$$

reading

$$H(x,t) = \exp[-t\widetilde{G}(x)\partial_x]x = F^{-1}[F(x)-t], \quad (2.20)$$

$$F(x) = \int^x dy/\widetilde{G}(y),$$

with F^{-1} being the inverse function, i.e., $F^{-1}[F(x)] = x$, and the quantity J stands for

$$J(x,t) \equiv \partial_x H(x,t) = \widetilde{G}[H(x,t)]/\widetilde{G}(x). \quad (2.21)$$

The resulting path integral representation converges very rapidly and takes *much* less single step iterations than either of the standard numerical routines described in the Appendix. One drawback of the method, however, is that obtaining numerical results valid to order $1/N^{2k}$ requires much larger computation than the corresponding (of the same order) path integral based on an analytic single step propagator. It may also be noted that in many dimensions, closed form expressions for $\mathbf{H}(\mathbf{q},t)$, like Eq. (2.20), are available for a few models and therefore approximate evaluation of the deterministic solution is generally required. For short times, this can be done rather accurately by expanding $\mathbf{H}(\mathbf{q},t)$ in a Taylor series about $t=0$ [7]. When applied to the present problem, the expansion reads

$$H(x,t) = x - t\widetilde{G}(x) + t^2\widetilde{G}(x)\widetilde{G}'(x)/2 + O(t^3), \quad (2.22)$$

$$J(x,t) = \exp[-t\widetilde{G}'(x) + t^2\widetilde{G}(x)\widetilde{G}''(x)/2] + O(t^3).$$

Hereby, the prime denotes differentiation with respect to x. It is clear that the use of approximations like Eq. (2.22) spoils the time reversibility of the single-step propagator, Eq. (2.8). This brings up an interesting question, which will be addressed in Sec. III: Does the use of Eq. (2.22) also spoil the enhanced error reduction?

B. Exponential power series expansion method

As we already noted, numerical higher-order propagators, although accurate, require larger computational effort than analytic propagators of the same order. For this reason, there has long been a desire to work out a simple computational

tool for generating analytic expressions for the propagator accurate to an order in τ as high as possible. Only very recently has such a theory been developed in terms of an exponential power series expansion formalism [8]. The theory differs from other perturbation techniques in that the time evolution operator is approximated by a global polynomial expansion valid not only for short times, but also in the intermediate- and long-time domain. This is achieved by representing the full propagator as a product of the reference propagator P_r with the configuration function

$$P(x,t|x_0) = P_r(x,t|x_0) \exp[W(x,x_0;t)], \qquad (2.23)$$

and expanding the exponent of the configuration function in a power series in a given function of t:

$$W(x,x_0;t) = \xi^{n-1}(t) W_n(x,x_0), \quad n \geq 1. \qquad (2.24)$$

Here, we restrict the discussion to the function $\xi(t)$ given by

$$\xi(t) = (1 - e^{-2rt})/2r, \qquad (2.25)$$

though a generalization to an arbitrary dependence ξ of t is also possible [8]. This particular time dependence has been chosen as it is associated with the width of the reference propagator, Eq. (2.18), and so it is expected to give a reasonable time scale in a general case. Then, inserting Eqs. (2.23) and (2.24) into Eq. (2.1) and equating like powers of ξ, we arrive at a hierarchy of linear inhomogeneous first-order differential equations for the expansion coefficients. These are solved analytically to yield the following explicit expressions for the first few coefficients:

$$W_1(x,x_0) = \int_{x_0}^{x} dy \, \widetilde{G}(y)/D,$$

$$W_2(x,x_0) = -\int_0^1 du \, V_2[x_0 + u(x-x_0)],$$
$$\qquad (2.26)$$
$$W_3(x,x_0) = r W_2(x,x_0) - D[2W_2(x,x_0) + V_2(x)$$
$$+ V_2(x_0)]/2(x-x_0)^2,$$

with

$$V_2(x) = \tfrac{1}{2}[G^2(x)/D + G'(x) - r^2 x^2/D + r]. \qquad (2.27)$$

The rest of the expansion coefficients W_n with $n \geq 4$ are obtained recursively by means of

$$W_n(x,x_0) = -\int_0^1 du \, u^{n-2} V_n[x_0 + u(x-x_0), x_0], \qquad (2.28)$$

where $V_n(x,x_0)$ is a known function determined in terms of lower-order terms

$$V_n = r V_{n-1} - r(n-2) W_{n-1} - (D/2) W''_{n-1}$$
$$- \sum_{j=2}^{n-2} [(D/2) W'_{n-j} - b_{n-j} x_0] W'_j, \qquad (2.29)$$

with b_n given by

$$b_n = r^n (2n-3)!!/n!.$$

Unfortunately, the recursive evaluation of the expansion coefficients does not allow us to express $W_n(x,x_0)$ in closed form and thus study general convergence properties for Eq. (2.24). Establishing these properties is a quite difficult task, which lies anyway outside the scope of the present paper, though experience with similar problems [20] suggests that the series in Eq. (2.24) is in general a divergent asymptotic one.

The above power series representation of the propagator is exact in the sense that no approximations have been made in order to derive it. The recursive evaluation of the expansion coefficients is carried out *systematically* to any desired order in $\xi(t)$ and allows one to *analytically* calculate the dynamics in the *whole* time domain [8]. Computer algebra manipulators can be used to do this very efficiently. One may thus expect that a truncation of the series in Eq. (2.24) at some low order $n = k + 1$ will provide us with a single step propagator

$$P_{(k)}(x,\tau|x_0) = P_r(x,\tau|x_0) \exp\left[\sum_{n=1}^{k+1} \xi^{n-1}(\tau) W_n(x,x_0)\right], \qquad (2.30)$$

which would be rather accurate not only for very short, but also for relatively large time steps τ. Its use in a path integral means that it will take considerably fewer integrations than the corresponding numerical propagator described in Sec. II A, to say nothing of the standard low-order propagators discussed in the Appendix. It may also be pointed out that the most commonly used approximation for the short time propagator, Eq. (B6), follows from Eq. (2.30) for $k = 1$ and $r = 0$ if one approximates the integral determining W_2, Eq. (2.26), by

$$W_2(x,x_0) = -\int_0^1 du \, V_2[x_0 + u(x-x_0)]$$

$$\approx \tfrac{1}{2}[V_2(x_0) + V_2(x)].$$

We note, however, that the above approach is not applicable to equations with singular diffusion matrices. Although there has been some recent success in describing the average of dynamical variables of these equations by expanding them in a power series in $\xi(t)$ [8], an analogous extension of the formalism on the propagator level is still lacking. Yet another disadvantage of the series representation is that the efficient evaluation of the propagator is feasible if and only if the coefficients of the Fokker-Planck equation are simple enough (polynomials or a finite sum of exponentials). In such a case, the various integrals involved in the expansion coefficients are to perform analytically. Otherwise, numerical quadratures are required, making Eq. (2.30) unsuited for path integral calculations.

C. Determination of the free parameter

Now it remains to determine the free parameter r appearing in the reference propagator, Eq. (2.17), so that the dynamics of the reference system resembles as closely as pos-

sible that of the full system. This is attainable if one minimizes in a least-squares sense the anharmonic correction, i.e.,

$$\partial_r \langle \widetilde{G}^2(x)[t] \rangle = 0, \tag{2.31}$$

which immediately yields

$$r(t) = -\langle xG(x)[t] \rangle / \langle x^2[t] \rangle. \tag{2.32}$$

The above approach is very simple to implement and also general in the sense that it can be applied to any quasilinear single step propagator. The averages $\langle \rangle$ are easily evaluated by Eq. (2.12) before the solution $P(x,t)$ is advanced to the next time level. One can still further simplify the determination of r by averaging over the equilibrium distribution, Eq. (2.3),

$$r_e = -\langle xG(x) \rangle_e / \langle x^2 \rangle_e. \tag{2.33}$$

With Eq. (2.33) we arrive at a reference propagator that reproduces well the long-time dynamics of the full system. A possible explanation for this is that Eq. (2.33) is a good approximation to the least nonvanishing eigenvalue of the Fokker-Planck operator

$$\lambda_1 \approx r_e. \tag{2.34}$$

The disadvantage of the approach is that the free parameter so determined is independent of the particular form of the short time propagator used, whereas our calculations performed on model systems show that each short time approximation $P_{(k)}$ has its own optimal value of r that may be a function of τ and t (see Sec. III of the present article as well as Ref. [8]).

Before closing we note that the variational approach to path integrals is not new. It was developed first by Feynman as early as 1972 [21]. In the last decade, a considerable improvement of Feynman's original technique has been put forward [22]. The basic idea of the refined treatment is to map a physical system described by a general potential energy function $V(\mathbf{q})$ onto a harmonic-oscillator reference system and to use the affiliated frequency as a variational parameter. This treatment can yield realistic finite temperature properties of quantum systems and it also requires much less computer time. The reader can easily verify that the methods outlined in Secs. II A and II B further improve the variational approach, while retaining its principal advantages.

III. NUMERICAL RESULTS

It is now our aim to test the relative efficacy of the new discrete path integral solutions and compare it with that of standard path integral representations. The latter are briefly outlined in the Appendix and include the histogram representation by Wehner and Wolfer [5], the Trotter splitting of the standard type as in quantum statistics [23,24], and higher-order approximations derived from the cumulant expansion for the short time propagator [9]. To simplify our comparison we shall employ below the free parameter r independent of time, though the use of the time-dependent criterion for determining $r(t)$, Eq. (2.32), is also feasible. As a test model, we first consider a one-dimensional process governed by Eq.

(2.1). This problem is simple enough to enable us to compare with numerically exact results obtained by other means. For instance, on the order of 100 basis functions are already sufficient to achieve machine accuracy in the basis set evaluation of the propagator almost in the whole time domain. As a second and more challenging example, we tackle the Kramers model of chemical reactions. The model is governed by a two-dimensional Fokker-Planck equation, whose diffusion matrix does not possess an inverse. In this case, obtaining numerically exact nonstationary solutions is in general a far from simple task, while closed-form analytic results are only available in the long time limit when the system approaches equilibrium.

A. Overdamped Brownian motion

In order to show that the present path integral solutions are efficient for any system regardless of whether the potential can be represented as a sum of harmonic and anharmonic terms, we first consider a one-dimensional model, Eq. (2.1), with a pure quartic potential given by

$$U(x) = \tfrac{1}{4} x^4. \tag{3.1}$$

We shall apply the various approximations discussed above for the short time propagator to the path integral evaluation of the second cumulant $M_2(t) = \langle\langle x^2(t) \rangle\rangle$. This quantity is determined by the first two moments of the Fokker-Planck equation, Eq. (C3), and characterizes the width of the distribution function $P(x,t)$. The calculations are performed for $D=1$ and $x_0=1$, with $\tau=0.1$. The method used to numerically evaluate Eq. (1.5) is described in Ref. [9]. A grid of 64 points in the interval $[-2.7, 2.7]$ was found to be sufficient for the quadrature. Finally, we compare with numerically exact results that are obtained by a basis set method [25].

To begin with, we illustrate the efficacy of the time-independent criterion for determining r suggested in Sec. II, Eq. (2.33). According to that criterion, an optimal value of the free parameter is $r_e = 1.04$. Our calculations, performed with the second-order Trotter-approximated propagator [Eq. (2.16)], reveal that the best choice of r is very close to the above estimation. This is evidenced by Fig. 1, which shows the relative error

$$\varepsilon = [(\text{approximate}) - (\text{exact})]/(\text{exact}) \tag{3.2}$$

in the path integral evaluation of the second cumulant made by using Eq. (2.16) as a function of t. The most accurate results are attained for $r=0.95$, which is nearly the first nonzero eigenvalue of the Fokker-Planck operator, $\lambda_1 = 0.967$.

For demonstrating the efficacy of Richardson's extrapolation technique, we fix $r=1$ and repeat the calculation with $\tau = 0.1$, 0.05, and 0.025. Then Eqs. (2.13) are employed to successively eliminate $1/N^2$ and $1/N^4$ errors. Figure 2 shows the resulting errors obtained with the Trotter single step propagator, Eq. (2.16), using the true deterministic solution, Eq. (2.20), and its Taylor series approximation, Eq. (2.22). The logarithmic plot clearly illustrates that each removal of an additional power of $1/N^2$ increases accuracy by nearly two orders of magnitude. An interesting (perhaps surprising) finding revealed in our calculations is that the time reversibility, Eq. (2.8), does not play the decisive role that has been
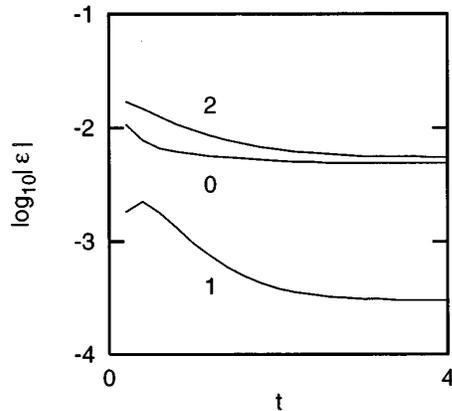
FIG. 1. Logarithm of the relative error $\log_{10}|\varepsilon|$, Eq. (3.2), in the path integral evaluation, with $\tau = 0.1$, of the second cumulant for a quartic potential [Eq. (3.1)] and for $x_0 = 1$ and $D = 1$ made by the quasilinear Trotter-approximated propagator, Eq. (2.16) with $r = 0, 1,$ and 2.

attributed to it by Schmidt and Lee [16]. The enhanced error reduction is seen to occur even though the single step propagator [Eqs. (2.16) and (2.22)] fails to satisfy Eq. (2.8) exactly. This is because the violations of the time reversibility
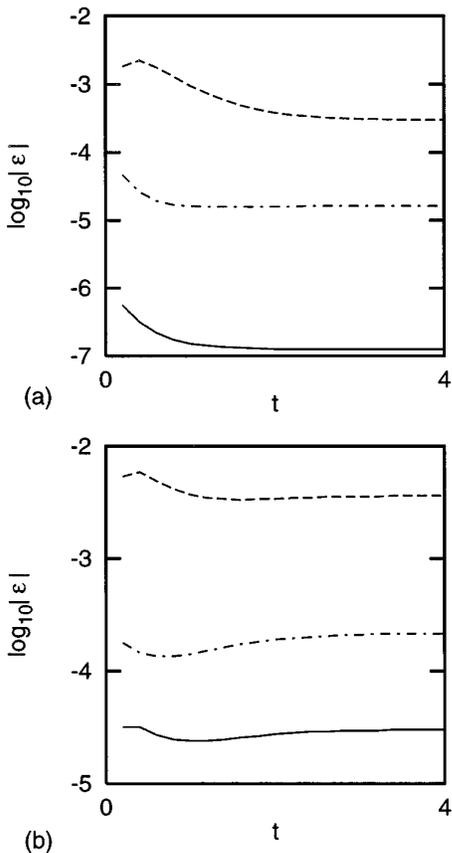
FIG. 2. Successive error reduction made by Eqs. (2.13). The dashed, dot-dashed, and solid lines are, respectively, for errors of order N^{-2}, N^{-4}, and N^{-6}. The results are obtained for $r = 1$ using the Trotter-approximated propagator, Eq. (2.16) with (a) the true deterministic solution [Eq. (2.20)], and (b) its Taylor series approximation [Eq. (2.22)].
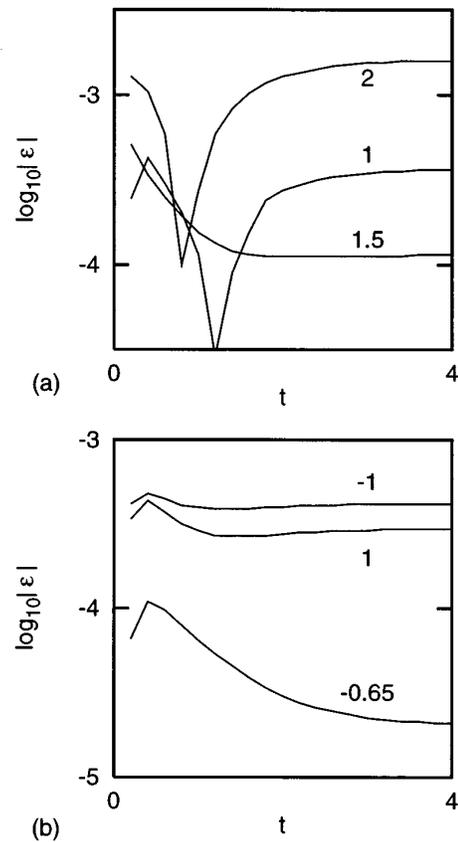
FIG. 3. Same as in Fig. 1, but for the short time propagator given by the power series, Eq. (2.30) with (a) $k = 2$ and (b) $k = 3$.

are of the same order as the error. Our finding is particularly important for multidimensional systems, as there is no closed-form expression for $\mathbf{H}(\mathbf{q}, t)$ in this case.

Next, we apply the short time propagators obtained by truncating the power series after the $k = 1, 2, 3,$ and 4 term, Eq. (2.30), to the path integral evaluation of the same quantity. In order to see the efficacy of these approximations as a function of the free parameter, we performed calculations over a wide range of r. We have found that for each value of the truncation number there is its own optimal value of r. This optimal value varies drastically from k to $k + 1$ and, in contrast to that given by Eq. (2.33), can become even negative. The latter is evidenced by Fig. 3, which shows errors obtained for $k = 2$ and 3. The bottom curves in the figure correspond to the best choice of r determined by computation. We have also found that for all considered k's the choice $r = 1$ [according to Eq. (2.33)], although good, is not the best. It should be stressed, however, that even with this (far from best) choice of r we are able to attain acceptable accuracy without *any* increase of computational effort solely by increasing the number of terms involved in the sum of Eq. (2.30). As is seen from Fig. 4, a precision of $10^{-4.5}$ is already achieved for $k = 4$. This is in contrast to the fourth-order Trotter-approximated propagator, which requires for comparable accuracy a computation that is three times as large (cf. Fig. 2). Finally, we note that in a wide range of r results obtained with $k = 2$ turn out to be very close to those of $k = 3$. One might thus expect that the extrapolation formula of Eq. (2.11) could also be very efficient in this case. Indeed,
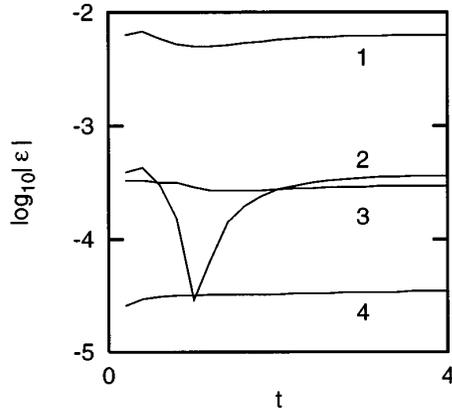
FIG. 4. Successive error reduction made by the power series short time propagator, Eq. (2.30) with $r=1$ and $k=1,\ 2,\ 3,$ and 4. The parameters are the same as in Fig. 1.

our calculations reveal that the use of Eq. (2.11) may increase accuracy by two and even three orders of magnitude. But this is not generally the case for higher-order extrapolations of Eqs. (2.13). Figure 5 shows errors made by using Eq. (2.30) for $r=1.5$ and $k=2$, and with an initial value of $\tau=0.1$. The solid curve in the figure clearly illustrates that application of Eqs. (2.13) to eliminate $1/N^4$ errors considerably decreases accuracy rather than to further increase it (cf. Fig. 2). This is because the propagator formed of N products of the power series approximations $P_{(2)}$, though more accurate than the Trotter-approximated propagator, does not generally have errors proportional to only powers of $1/N^2$.

Finally, in Fig. 6 we plot the errors made by the various second-order quasilinear approximations for the short time propagator, Eqs. (2.16), (2.30), and (C4). Each of these approximations is taken with its own best choice of r determined by computation. Also shown are the errors made by the standard short time propagators based on a free-particle reference system, Eqs. (1.6) and (B6). As seen in the figure, the primitive short time approximation of Wehner and Wolfer [Eq. (1.6)] can at best reduce the error to a few percent, being thus the worst of the considered propagators. This is not surprising, as Eq. (1.6) follows from the cumulant expansion for the propagator, Eq. (C4), truncated at $k=1$ for
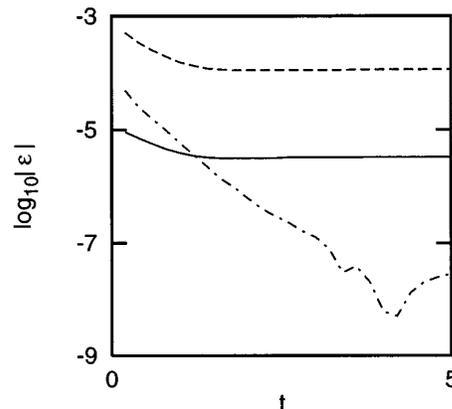
FIG. 5. Same as in Fig. 2, but for the short time propagator given by the power series, Eq. (2.30) with $k=2$ and $r=1.5$.
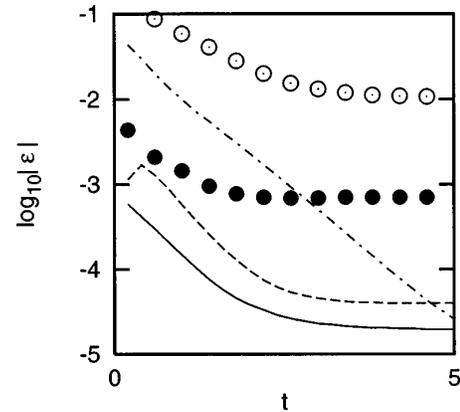
FIG. 6. Errors made by using various short time approximations. The parameters are the same as in Fig. 1. Open circles: propagator of Wehner and Wolfer, Eq. (1.6); solid circles: standard Trotter formula, Eq. (B6); dashed line: quasilinear Trotter approximation, Eq. (2.16) with $r=0.95$; dot-dashed line: cumulant expansion, Eq. (C4) with $k=2$ and $r=1.5$; solid line: power series expansion, Eq. (2.30) with $k=2$ and $r=1.55$.

$r=0$. Being truncated at $k=2$ for $r=1.5$, the cumulant expansion of the short time propagator reduces the error by nearly one order of magnitude. But the error still remains rather large in the initial time regime. Although no linear reference system is used in the standard Trotter formula [Eq. (B6)], the effect of preserving time reversibility is also the reduction of the error by one order of magnitude. The present quasilinear second-order propagators are seen to further reduce the error roughly by a factor of 14. It should be pointed out that the more accurate description is achieved without *extra* computational effort solely due to the proper choice of the reference system. In contrast, a precision of five significant digits is attainable with the standard Trotter-formula method, Eq. (B6), just for $\tau \lesssim 0.03$. While the method of Wehner and Wolfer fails to reach this level of accuracy even though $\tau = 0.001$.

Next, we apply the same techniques to the dynamics of a bistable system given by

$$U(x) = -\tfrac{1}{2}x^2 + \tfrac{1}{4}x^4. \tag{3.3}$$

This example is more challenging in that for $D \ll 1$ the first nonzero eigenvalue of the Fokker-Planck operator becomes exponentially small

$$\lambda_1 = O(e^{-1/2D}). \tag{3.4}$$

Consequently, simulations over very long times are required to describe all regimes of interest, reaching from fast intrawell relaxation ($t \gg \lambda_2^{-1} \approx 1$) to slow interwell equilibration ($t \gg \lambda_1^{-1}$). In such a case, the standard way of reducing errors of time discretization by decreasing τ will substantially increase the necessary computational effort and, therefore, higher-order propagators are generally desirable. To be specific, we restrict our discussion to a moderately small value of the diffusion coefficient, $D=0.1$. The calculation is performed for $\tau = 0.2$ and $x_0 = -1$ on a grid of 64 points in
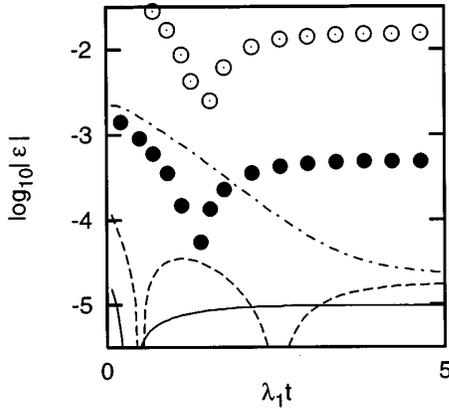
FIG. 7. Same as in Fig. 6, but for a double well, Eq. (3.3), and for $D=0.1$, with $\tau=0.2$. Open circles: propagator of Wehner and Wolfer, Eq. (1.6); solid circles: standard Trotter formula, Eq. (B6); dashed line: fourth-order Trotter-approximated propagator, Eqs. (2.11) and (2.16) with $r=0$; dot-dashed line: cumulant expansion, Eq. (C4) with $k=4$ and $r=-0.35$; solid line: power series expansion, Eq. (2.30) with $k=3$ and $r=-0.25$.

the interval $[-1.7,1.7]$. Equation (2.33) gives in this case $r_e=0.05$, which is close enough to the least nonvanishing eigenvalue $\lambda_1=0.00277$.

We again performed calculations with the two methods described in Sec. II for different values of the free parameters r. Since the conclusions drawn in this case are essentially the same as for the pure quartic oscillator we do not present these results. We only compare in Fig. 7 the accuracy of the various approximations discussed above for the single-step propagator. As expected, the power series expansion turns out to be the most efficient method. The error made by Eq. (2.30) for $k=3$ is seen to be even lower than that of the fourth-order Trotter-approximated propagator that is constructed with Eq. (2.16) using the extrapolation of Eq. (2.11) to eliminate quadratic errors. The latter in turn is more accurate than the fourth-order cumulant expansion. It is also seen that the error made by the standard Trotter formula, Eq. (B6), is nearly two orders of magnitude larger than the errors made by the present methods. It may be noted here that a precision of 10^{-5} is achievable in calculations with Eq. (B6) only for $\tau\sim0.05$, i.e., with substantial increase of computational effort. The error made by the method of Wehner and Wolfer is again much larger than those of the other techniques.

B. Kramers model

As a second example, we consider the original Kramers model, which consists of a unit mass particle in a potential $U(x)$, driven both by linear friction with coefficient γ and by thermal noise of temperature β^{-1} [26]. The dynamics is governed by the two-dimensional Fokker-Planck equation for the probability density of finding the particle at time moment t at position x with velocity v

$$\partial_t P(x,v,t)=[-v\partial_x+U'(x)\partial_v+\gamma\partial_v(v+\beta^{-1}\partial_v)]P(x,v,t). \tag{3.5}$$

It is not hard to check by direct substitution that the stationary solution of Eq. (3.5) has the standard Maxwell-Boltzmann form

$$P_s(x,v)=Z^{-1}\exp[-\beta v^2/2-\beta U(x)]. \tag{3.6}$$

After integration over v it reduces to Eq. (2.3) with $D=2\beta^{-1}$. The above model, although simple, is of enormous utility in understanding and evaluating the influence of the medium on dynamical processes. It is commonly used in studies of superionic conductors, Josephson tunneling junctions, nonlinear optics, nucleation, and escape rate theories [27]. The essential features of many of these processes mimic the dynamics of potential barrier crossing, a problem that was first treated by Kramers in his seminal paper [26].

To be specific we choose a symmetric bistable potential of the form

$$U(x)=E(x^2-1)^2, \tag{3.7}$$

with E being the height of the potential barrier. This example is particularly challenging for several reasons. First, the least nonvanishing eigenvalue of the Fokker-Planck operator is exponentially small, $\lambda_1=O(e^{-\beta E})$. But this is not the only reason that may require simulations over very long times. Long time length simulations are also necessary in the weak damping limit, $\gamma\gg1$, even though the potential barrier is rather small, $\beta E\lesssim1$. In such a case, the energy of the particle is an almost conserved quantity, and the particle undergoes many oscillations between the stable states until it thermalizes in one of them. Second, Eq. (3.5) cannot be cast into a Hermitian form, as its diffusion matrix is singular. The latter property is an obstacle for employing the efficient series representation technique, outlined in Sec. II B, and also prevents us from making use of powerful nonperturbative schemes of quantum mechanics. Standard numerical methods such as basis set expansions could be efficient in studying dynamical properties of Eq. (3.5) in the intermediate and long time regimes provided that the desired level of accuracy is just a few percent. Otherwise, on the order of 40–50 basis functions per variable are necessary for a precision of 10^{-6} and this limits the practical applicability of the approach to very long times, i.e., to the cases where the first two eigenvalues form the main contribution to the transition probability. Finally, the second cumulant of the variable x tends to zero as [9]

$$\langle\langle x^2\rangle\rangle=\tfrac{2}{3}\gamma\beta^{-1}\tau^3+O(\tau^4), \tag{3.8}$$

rather than linearly as is the case for processes with invertible diffusion matrices, Eq. (1.8). This means that with $\tau\to0$ the propagator of Eq. (3.5) rapidly degenerates into a delta function, requiring very fine spatial discretization. In such a case, the standard way of reducing errors by decreasing τ will substantially increase the storage requirements and execution time necessary to get good resolution in path integral calculations.

The above observations are in drastic contrast to the Trotter-formula method outlined in Sec. II A, which allows one to get very accurate results without using large dimensional matrices. It is an approach that can be applied to simple and complex systems and singularity of the diffusion matrix does not present special problems. In particular, when applied to Eq. (3.5), it yields a second-order propagator of the form [7]

$$P_{(2)}(x,v,\tau|x_0,v_0) = P_{OU}[x,v - \tau\widetilde{G}(x)/2,\tau|x_0,v_0$$

$$+ \tau\widetilde{G}(x_0)/2], \qquad (3.9)$$

where $\widetilde{G}(x) = rx - U'(x)$, while the reference propagator $P_r(x,v,\tau|x_0,v_0)$ is defined by

$$B = -v\partial_x + rx\partial_v + \gamma\partial_v(v + \beta^{-1}\partial_v). \qquad (3.10)$$

An explicit expression for P_r can be found in Ref. [2]. An accurate description of dynamical properties is attainable with Eq. (3.9) in all regimes of practical interest with relatively large time steps τ thanks to the numerical efficiency of the enhanced error reduction techniques. In order to illustrate this statement, we have calculated the stationary solution $P_e(x)$ for different values of β, γ, x_0, and v_0 on a 64 $\times 64$ (x,v) grid in the intervals $|x| \leq 2$ and $|v| \leq 6$. The quadrature of Eq. (1.5) are evaluated iteratively by taking advantage of the fast Fourier transform (FFT). Although path integral representations of stochastic dynamics are, in general, not suited to the FFT, a way for overcoming this problem has been developed in a previous paper [17]. The method employs the Stirling interpolation to dynamically readjust the distribution function every time step with a mild increase in cost and with no loss of precision.

Since except for the Trotter-formula method (Sec. II A) and the cumulant expansion (Appendix C), the rest of the discussed path integral approaches are not applicable to Eq. (3.5), results of only these two methods are presented in Fig. 8. The figure is a plot of the relative errors obtained in $P_e(x)$ for $\beta = 1$, $E = 5$, with $r = 0$. As anticipated, these results appear to be independent of the initial conditions and friction coefficient. We note the relatively easy way by which an acceptable accuracy of 10^{-6} is achieved in terms of the present Trotter-approximated propagator with discretizations $\tau = 0.1$, 0.05, and 0.025 using Eq. (2.13) to remove quadratic and quartic errors. It is also important that the accuracy of the method is rather insensitive to γ almost in all regimes of physical interest ranging from the underdamped Brownian motion, $\gamma \ll 1$, to the spatial diffusion regime, $\gamma \gg 1$. The same, however, is not true for the cumulant expansion method (a generalization of the method to many dimensions can be found in Ref. [9]). Although its accuracy, for $\tau = 0.1$, is seen to be comparable with that of the Trotter-formula method, the utility of the propagator obtained by truncating the cumulant expansion turns out to be very restrictive with respect to the friction coefficient. This is because any finite-order truncation of the cumulant expansion fails to provide the positivity of the second cumulants for all τ, γ, x_0, and v_0 at once. For each τ the latter become negative with increasing γ, and very short time steps are required to overcome this problem.

IV. CONCLUDING REMARKS

At present there exist several theoretical approaches to constructing path integral representations for Fokker-Planck dynamics. Their mutual correspondence, however, is complicated. This paper is an attempt to put the approaches in order. We briefly summarize and review much of what has been done before in this field with the aim to compare the
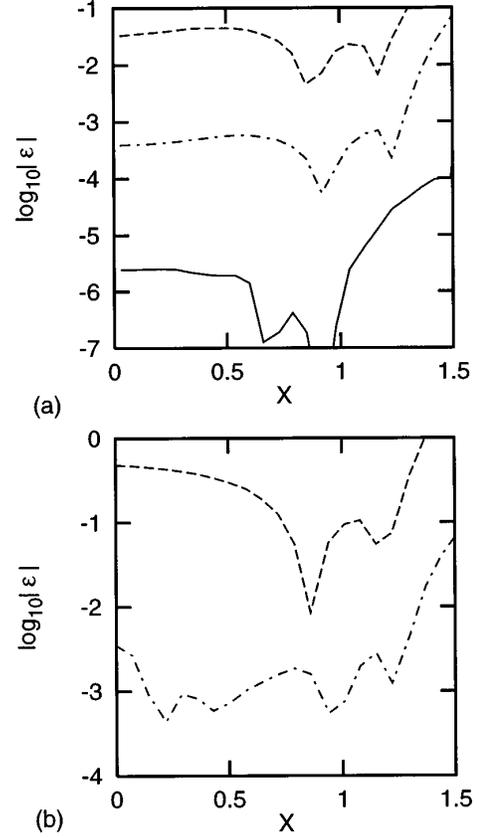
FIG. 8. Successive error reduction in the path integral evaluation of the stationary solution of a Kramers model, Eqs. (3.5) and (3.7) with $\beta E = 5$. The dashed, dot-dashed, and solid lines are, respectively, for errors of order $1/N^2$, $1/N^4$, and $1/N^6$. (a) Trotter-approximated propagator, Eqs. (3.9) and (2.13); (b) cumulant expansion.

relative efficacy of different path integral representations available in the literature. Each of these representations has its own advantages and drawbacks. Specific advantages sought include having a rapid convergence rate, being easy to implement, and requiring a small amount of modification when the Fokker-Planck coefficients are changed. From this point of view, the approach recently introduced by one of us [8,17] (A.N.D.) is particularly interesting. Its key idea is to treat a general Fokker-Planck process as a perturbation of a reference Ornstein-Uhlenbeck process, and to then use perturbation techniques to quantify what is missing from the reference description. We have shown that the representations so obtained are both theoretically and numerically advantageous with respect to other path integral representations now in use in the sense that they give much more accurate results with a little computation. It is particularly pleasing that high accuracy is achievable with the present technique even though the time step τ is rather large. A substantial reduction of errors is attained by appropriately choosing the free parameter r and/or by increasing the order of approximation k. The examples discussed in Sec. III are very encouraging in this regard. In contrast, the accuracy of the standard path integral representations is controlled only by increasing the number of integration variables N.

As anticipated, the accuracy of the power series method,

Eq. (2.30), appears to be more favorable than that of the other techniques, if the criterion is solely accuracy for a given time step τ. We recognize, however, that this is not the only aspect when discussing the power series propagator versus, e.g., the standard Trotter formula, Eq. (B6). The latter is more easily implemented due to its very simple structure, while the former involves the various integrals whose evaluation may require a more analytical work. On the other hand, both the power series expansion technique and the standard Trotter-formula method fail to treat processes with singular diffusion matrices. In view of the above remark, the present Trotter-approximated propagator [Eq. (2.16)] seems preferable. Being structurally similar to the standard Trotter approximation, it nevertheless shows a dramatic improvement over the latter in that it is applicable to an arbitrary stochastic process and requires considerably less integrations for achieving a given precision.

ACKNOWLEDGMENTS

APPENDIX A: HISTOGRAM REPRESENTATION OF WEHNER AND WOLFER

Wehner and Wolfer [5] developed their iterative path integral method using Eqs. (1.5) and (1.6), and the Gaussian nature of the postpoint variables. The method is based on a histogram representation of the distribution function and reduces the problem of numerically solving the Fokker-Planck equation to simple matrix vector multiplications,

$$P_i(t+\tau) = T_{ij}(\tau)P_j(t), \quad 1 \le i, \ j \le M, \qquad (A1)$$

where $P_i(t) = P(x_i, t)$, and where the elements of the transition matrix T_{ij} are evaluated on a grid of M points, $x_i = x_1 + (i-1)h$, by numerical quadratures

$$T_{ij}(\tau) = \frac{1}{h} \int_{x_i-h/2}^{x_i+h/2} dx \int_{x_j-h/2}^{x_j+h/2} dy \, P_{(1)}(x,\tau|y). \qquad (A2)$$

However, the primitive single step propagator used by Wehner and Wolfer, Eq. (1.6), fails to treat processes with non-invertible diffusion matrices and requires very short time increments for accuracy. Accordingly, the dimension of the resulting integral and, therefore, the number of matrix vector multiplications can be very high if the desired propagation time is long. Moreover, the number of matrix elements to be stored as well as the execution time necessary for each matrix vector multiplication grow exponentially with the dimensionality of the system. This makes the above propagation scheme rather impractical for systems with more than one degree of freedom. Recent applications of the method in neuroscience studies have shown how difficult it can be even in two dimensions to get good resolution because of CPU constraints [6].

APPENDIX B: FAST FOURIER TRANSFORM METHOD

A major step forward was the introduction of efficient grid methods, such as those based on the FFT [23]. When applied to stochastic dynamics, high proficiency is usually achieved by making use of an apparent analogy between the Fokker-Planck equation for the probability density function and the Bloch equation for the coordinate density matrix [24]. This analogy always exists for one-dimensional systems; but it is not a generic case in many dimensions. Multidimensional stochastic dynamics, Eq. (1.1), can be cast into the Hermitian form

$$\partial_t \psi(\mathbf{q},t|\mathbf{q}^0) = -\mathcal{H}\psi(\mathbf{q},t|\mathbf{q}^0) \equiv [\tfrac{1}{2}D_{ij}\partial_{ij}^2 - V(\mathbf{q})]\psi(\mathbf{q},t|\mathbf{q}^0), \qquad (B1)$$

if and only if the Fokker-Planck operator obeys strict detailed balance, i.e. [2],

$$L(P_e f) = P_e L^+ f \qquad (B2)$$

for any smooth function f, where L^+ denotes the backward operator

$$L^+ = G_i(\mathbf{q})\partial_i + \tfrac{1}{2}D_{ij}\partial_{ij}^2, \qquad (B3)$$

while P_e is the equilibrium distribution satisfying $LP_e = 0$. In such a case, the auxiliary quantity $\psi(\mathbf{q},t|\mathbf{q}^0)$ is associated to the propagator $P(\mathbf{q},t|\mathbf{q}^0)$ by means of the ansatz

$$P(\mathbf{q},t|\mathbf{q}^0) = \sqrt{P_e(\mathbf{q})/P_e(\mathbf{q}^0)}\,\psi(\mathbf{q},t|\mathbf{q}^0), \qquad (B4)$$

while the potential $V(\mathbf{q})$ is determined in terms of the drift coefficients G_i and the inverse diffusion matrix D^{ij} by

$$V(\mathbf{q}) = \tfrac{1}{2}[D^{ij}G_i(\mathbf{q})G_j(\mathbf{q}) + \partial_i G_i(\mathbf{q})]. \qquad (B5)$$

If Eq. (B2) does not hold, a mathematical obstacle exists to applying by analogy the quantum principles because the Fokker-Planck operator is generally non-Hermitian.

Path integral methods of the standard type as in quantum statistics have been employed in special cases where L can be transformed to a Hermitian form [24]. The most common procedure of approximating the propagator for short time τ utilizes the symmetric Trotter splitting of the time evolution operator, which is based on partitioning the Hamiltonian into kinetic and potential energy terms [10,24]. When applied to one-dimensional systems, this yields a second-order short time propagator with a free-particle reference system reading

$$\psi_{(2)}(x,\tau|x_0) = (2\pi\tau D)^{-1/2}\exp\{-(x-x_0)^2/2\tau D$$
$$- \tau[V(x)+V(x_0)]/2\}. \qquad (B6)$$

With Eq. (B6), the expression for a single iteration becomes well suited to the FFT,

$$P(x,t+\tau)=(2\pi)^{-1}\exp[-U(x)/D-\tau V(x)/2]\int_{-\infty}^{\infty}dz$$

$$\times\exp(-izx-\tau Dz^2/2)\int_{-\infty}^{\infty}dy$$

$$\times\exp[izy+U(y)/D-\tau V(y)/2]P(y,t). \tag{B7}$$

The resulting propagation scheme is obviously efficient in terms of storage requirements, as no transition matrix is involved in calculations. In addition, the favorable scaling of the fast Fourier transform, which is almost *linear* with the number of coupled degrees of freedom [19], allows for much more rapid evaluation of the integrals in Eq. (1.5) than matrix multiplication techniques. The main disadvantage of the method is that it is based on the primitive (free-particle, low-order) short time propagator which cannot be applied to systems without strict detailed balance.

APPENDIX C: CUMULANT GENERATING FUNCTION FORMALISM

Yet another way to construct higher-order analytic approximations for the propagator is to make use of the cumulant generating function formalism [9]. The key points of the method are representing the propagator in the form

$$P(x,t|x_0)=(2\pi)^{-1}\int_{-\infty}^{\infty}dz\exp[-ixz+\varphi(z)], \tag{C1}$$

and expanding the generating function $\varphi(z)$ in a power series,

$$\varphi(z)=i^n M_n z^n/n!, \tag{C2}$$

where the quantities M_n, which are called the cumulants of the variable x, are expressible in terms of moments

$$M_1=\langle x\rangle, \quad M_2=\langle x^2\rangle-\langle x\rangle^2,$$
$$M_3=\langle x^3\rangle-3\langle x\rangle\langle x\rangle^2+2\langle x\rangle^3, \quad \dots . \tag{C3}$$

An explicit general formula for converting moments into cumulants can be found in Ref. [1]. It should be noted here that both cumulants and moments are functions of the prepoint x_0 and the time increment τ, but to keep the notation simple we do not indicate this explicitly. When the cumulants M_n are all determined, the Fourier inversion formula (C1) gives the propagator $P(x,t|x_0)$ for an arbitrary net increment t. As, however, we are interested in the short time dynamics, a truncated cumulant expansion can be used to determine the short time propagator

$$P_{(k)}(x,\tau|x_0)=(2\pi)^{-1}\int_{-\infty}^{\infty}dz\exp\left[iz(M_1-x)-\tfrac{1}{2}M_2z^2\right.$$
$$\left.+\sum_{n=3}^{k}M_n(iz)^n/n!\right]. \tag{C4}$$

In deriving the above expression we have used that [9]

$$M_1=x_0+O(\tau), \quad M_2=O(\tau), \quad M_n=O(\tau^n) \ (n>2). \tag{C5}$$

The cumulants involved in Eq. (C4) are to be evaluated up to and including terms of order τ^k. This can be done by expanding the formal solution for moments

$$\langle x^n(t)\rangle=[e^{tL^+}x^n]_{x_0}$$

in a Taylor series in t [9]. Here we outline an alternative method which allows us to construct an expansion for cumulants by treating a general Fokker-Planck process as a perturbation of an Ornstein-Uhlenbeck process. To this end, we again split the full drift coefficient into a linear part $G_r(x)=-rx$ and the rest $\widetilde{G}(x)=G(x)+rx$, and integrate the moments equations of motion from $t=0$ to $t=\tau$,

$$\langle x^n(\tau)\rangle=e^{-nr\tau}x_0+n\int_0^{\tau}ds\,e^{nr(s-\tau)}$$

$$\times\langle\{x^{n-1}\widetilde{G}(x)+\tfrac{1}{2}(n-1)Dx^{n-2}\}(s)\rangle. \tag{C6}$$

Explicit expressions for the moments can then be obtained by expanding the integrand of Eq. (C6) in a Taylor series about the prepoint x_0. Repeated iteration of the resulting equations, while neglecting terms of order higher than τ^3, gives the following expressions for the first few cumulants:

$$M_1=x_0+a_1(\tau)G_0+a_2(\tau)G_0\widetilde{G}_0'+a_1^2(\tau)DG_0''/4$$
$$+a_3(\tau)G_0\widetilde{G}_0'^2+a_4(\tau)(2G_0^2+3D\widetilde{G}_0')G_0''$$
$$+a_5(\tau)DG_0G_0'''+a_6(\tau)D^2G_0^{IV},$$

$$M_2=D[\tfrac{1}{2}a_1(2\tau)+a_1^2(\tau)\widetilde{G}_0'+a_7(\tau)\widetilde{G}_0'^2+4a_5(\tau)G_0G_0''$$
$$+8a_6(\tau)DG_0'''],$$

$$M_3=(1-6e^{-2r\tau}+8e^{-3r\tau}-3e^{-4r\tau})D^2G_0''/4r^3, \tag{C7}$$

where $F_0=F(x_0)$, $F=G,G',\dots$, and the expansion coefficients are

$$a_1(\tau)=(1-e^{-r\tau})/r,$$

$$a_2(\tau)=[1-(1+r\tau)e^{-r\tau}]/r^2,$$

$$a_3(\tau)=[1-(1+r\tau+\tfrac{1}{2}r^2\tau^2)e^{-r\tau}]/r^3,$$

$$a_4(\tau)=(1-2r\tau e^{-r\tau}-e^{-2r\tau})/4r^3,$$

$$a_5(\tau)=[2-(3+2r\tau)e^{-r\tau}+2e^{-2r\tau}-e^{-3r\tau}]/8r^3,$$

$$a_6(\tau)=(3-8e^{-r\tau}+6e^{-2r\tau}-e^{-4r\tau})/96r^3,$$

$$a_7(\tau)=[3-4(1+r\tau)e^{-r\tau}+(1+2r\tau)e^{-2r\tau}]/2r^3. \tag{C8}$$

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. The calculations are doable *analytically regard-*

less of the specific form of the drift and diffusion coefficients, thus permitting one to get accurate results with minimal computational effort. At first sight we arrive, with these developments, at a powerful high-accuracy method that is efficient in terms of speed and storage requirements, simultaneously. Indeed, the calculations we have performed on model systems show that the method is accurate for very short time steps τ if one truncates the series in Eq. (C4) at high enough order k. With increasing τ, however, the error begins to grow very rapidly, and beyond some τ_{max} that is noticeably smaller than unity, the method fails to produce correct results. This is because the range of validity of Eq. (C4) is restricted by the inequality $M_2 > 0$, which is satisfied only in the limit $\tau \to 0$. It is not hard to prove that this is generally true for any finite-order truncation of the cumulant expansion, Eq. (C4) [28].

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