

## Operator expansions in stochastic dynamics

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Higher-order operator factorizations are a powerful tool for efficiently treating classical mechanics. This paper presents an application of the method to stochastic dynamics. Using a fourth-order symmetric decomposition of the time evolution operator, we arrive at a high-accuracy scheme for propagating the distribution function in time. Its power is demonstrated by means of two problems, namely, the dynamics of a colored noise process and a Brownian particle in a potential field. The applications show our method to be superior over the standard propagation scheme based on the Trotter splitting in that it allows *much larger* time steps with *no loss* of precision. [S1063-651X(98)00902-7]

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### I. INTRODUCTION

Recent years have seen considerable activity in numerical methods that employ various different operator expansions to carry out calculations in quantum and statistical mechanics [1–9]. The key features of the methods are factorizing the time evolution operator into a product of  $N$  exponential operators,

$$e^{tL} = (e^{tL/N})^N, \quad (1.1)$$

partitioning the full operator  $L$  into two exactly solvable parts  $L = A + B$ ; and approximating the propagator for a short time  $\tau = t/N$  by a product of functions involving  $A$  and  $B$ ,

$$e^{\tau(A+B)} = S_k(\tau) + O(\tau^k), \quad (1.2)$$

where  $k$  denotes the order of approximation. The solution for an arbitrary long time  $t = N\tau$  is obtained by repeatedly using Eq. (1.2),

$$e^{t(A+B)} = S_k(t) + O(t^{k+1}/N^k), \quad S_k(t) = S_k(\tau)^N, \quad (1.3)$$

which in a coordinate representation yields the discrete path integral representation

$$P(\mathbf{q}, t) = \int \prod_{n=0}^{N-1} d\mathbf{q}^n P_k(\mathbf{q}^{n+1}, \tau | \mathbf{q}^n) P(\mathbf{q}^0, 0) + O(t^{k+1}/N^k), \quad (1.4)$$

with  $\mathbf{q}^N = \mathbf{q}$ . It is clear that the efficacy of the resulting propagation scheme depends crucially on the number of time discretizations (integration variables) necessary for convergence. The latter in turn can be reduced if the accuracy of the short time propagator  $P_k(\mathbf{q}^{n+1}, \tau | \mathbf{q}^n) = \langle \mathbf{q}^{n+1} | S_k(\tau) | \mathbf{q}^n \rangle$  can be extended to a longer time interval  $\tau$ .

The most common procedure of approximating the propagator for short time utilizes the Trotter splitting [1]

$$S_2(\tau) = e^{\tau A/2} e^{\tau B} e^{\tau A/2}. \quad (1.5)$$

A small sample of this work can be found in Refs. [2–4]. Since, however,  $A$  and  $B$  are in general noncommuting operators, the error accumulated in Eq. (1.4) by making use of this decomposition is of order  $1/N^2$ ; accordingly, the dimension of the resulting integral can be very high if the desired propagation time is long. A superior breakup was given by Suzuki [5], who proposed a generalization of Eq. (1.5) in the form

$$S_k(\tau) = \prod_i e^{a_i \tau A} e^{b_i \tau B}, \quad (1.6)$$

with coefficients  $(a_i, b_i)$  determined by the required order of accuracy. Although factorizations of arbitrarily high orders can be obtained in this way, the approach has no impact on solving many-body problems in quantum statistics and non-equilibrium statistical mechanics. The reason is that, beyond second order, any factorization of the form (1.6) must produce some negative coefficients in the set  $(a_i, b_i)$ . When applied to Fokker-Planck and/or Bloch equations, this means that negative times must appear at some diffusion operators, making the resulting factorization unbounded.

Some recent advance in this area can be attributed to the introduction of extrapolation methods to remove time slices errors in Trotter-approximated propagators [6,7]. An attractive feature of symmetric decompositions is that an approximate propagator constructed of  $N$  products, each of which is time reversible,

$$S_k(-t)S_k(t) = 1, \quad (1.7)$$

has an asymptotic error expansion with *even* powers of  $1/N$ . Therefore, standard extrapolation methods can be used successively to eliminate the low-order errors resulting from time discretization. In particular, a Romberg-type operator approximation without the  $1/N^2$  error is [6]

$$S_4(t) = \frac{1}{3}[4S_2(t/2N)^{2N} - S_2(t/N)^N]. \quad (1.8)$$

Implementing this numerically requires up to three times as much computation and doubles the storage, but the remaining error is of order  $1/N^4$ .

In the present paper we propose an alternative propagation scheme which provides the same level of accuracy *with*

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no increase of storage and computation. This is achieved by making use of a fourth-order symmetric factorization of the form

$$S_4(\tau) = e^{a\tau A} e^{\tau B/2} e^{\tau C} e^{\tau B/2} e^{a\tau A}, \quad (1.9)$$

with

$$C = (1 - 2a)A + \frac{1}{24}\tau^2[2(1 - 6a + 6a^2)A + (1 - 6a)B, [B, A]], \quad (1.10)$$

where  $a$  is an arbitrary number from the interval  $[0, 1]$ . The above breakup is obtainable by a variety of methods, e.g., by repeated application of the Baker-Campbell-Housdorff formula. It is a straightforward generalization of the various decompositions available in the literature for the exponential operator. In particular, a known decomposition of De Raedt and De Raedt [1] follows from Eqs. (1.9) and (1.10) with  $a = \frac{1}{2}$ ; while for  $a = \frac{1}{6}$  and  $a = (1 - 1/\sqrt{3})/2$ , it reproduces two different factorizations recently derived by Suzuki [8] (see also Ref. [9]).

Although approximations like Eq. (1.9) have been known since the early days [10], and have frequently been used for numerically solving many-body problems in classical mechanics, their effective application to Fokker-Planck dynamics has not yet been fully realized. A reason for this seems to be the impression that the commutator involved in Eq. (1.10) complicates the expression in such a way that the calculation of  $P_4$  is *always* out of the question. Indeed, applying the above factorization to simple one-dimensional systems, we immediately run into trouble, as the operator  $C$ , which arises in that case, is much more complicated than the original Fokker-Planck operator. The same, however, is not generally true for systems with more than one degree of freedom. The essential step in devising the method outlined below was to realize that application of Eq. (1.9) to multidimensional systems may be much easier than in one dimension. The necessary condition for this is the noninvertibility of the diffusion matrix. In such a case, use of Eq. (1.9) may be as simple as that of the primitive Trotter splitting, Eq. (1.5), and require no additional analytical work to evaluate the propagator.

It is our purpose here to illustrate the computational utility of that method in two concrete models: the dynamics of a colored noise process, and the Brownian motion in a potential field. For simplicity, in Eq. (1.10) we remove one of the two composite operators by setting  $a = \frac{1}{6}$ ,

$$C = \frac{2}{3}A + \frac{1}{72}\tau^2[A, [B, A]], \quad (1.11)$$

though other values of  $a$  are also possible. In particular, when evaluating both composite operators is not a major problem, the free parameter  $a$  can be determined according to some variational principles, so that the resulting short time propagator is accurate for as long a time  $\tau$  as possible. Moreover, since the breakup (1.9) is symmetric, extrapolation methods can be employed to improve its accuracy further. For example, an operator without the  $1/N^4$  error is

$$S_6(t) = \frac{1}{15}[16S_4(t/2N)^{2N} - S_4(t/N)^N]. \quad (1.12)$$

Finally, to conclude this introduction, it should be noted that there are also other methods for obtaining high-accuracy

short time propagators. We mention specifically the work of Drozdov [11], who developed a theoretical approach to approximate the single step propagator systematically by analytic expressions. The approach distinguishes itself from other methods in that it gives global approximations valid not only for short times, but also in the intermediate and long time domains. This is achieved by expanding the exponent of the propagator in a Taylor series in time, and efficiently extrapolating the behavior of the series to its eventual sum by means of sum acceleration techniques. As given, though, the approach applies only to Fokker-Planck processes whose diffusion matrices possess an inverse, and not to processes with singular diffusion matrices. Another useful approach is the cumulant expansion for the short time propagator [12], which also has an effect of reducing the number of integration variables. Various order approximations can either be derived from the underlying Langevin equations, or by solving time evolution equations of moments. The approach is simple and easily applicable to any Fokker-Planck equation regardless of whether or not the diffusion matrix is invertible; but the utility of the approximations so obtained is in general restricted to short times.

## II. SYSTEM DRIVEN BY COLORED NOISE

Over recent years, there has been a steadily growing interest in the effects that arise from colored noise in nonlinear dynamical systems [13]. A typical model repeatedly studied within this context is described by the stochastic differential equation

$$\dot{x} = G(x) + v(t), \quad (2.1)$$

where  $G(x)$  is an arbitrary function of  $x$ , and  $v(t)$  an external Gaussian stochastic force normalized to

$$\langle v(t) \rangle = 0, \quad \langle v(t)v(s) \rangle = \gamma D \exp(-\gamma|t-s|), \quad (2.2)$$

with  $\gamma^{-1}$  being the correlation time of the noise, and  $D$  the noise intensity. The statistics of systems (2.1) and (2.2) may be embodied in the two-dimensional Fokker-Planck equation

$$\begin{aligned} \partial_t P(x, v, t) &= LP(x, v, t) \\ &\equiv \{-\partial_x [G(x) + v] \\ &\quad + \gamma \partial_v (v + \gamma D \partial_v)\} P(x, v, t). \end{aligned} \quad (2.3)$$

One notes that the diffusion matrix of Eq. (2.3) does not possess an inverse, and the equation itself does not obey detailed balance. The former property prevents us from making use of many powerful nonperturbative schemes of quantum and statistical mechanics, while the latter means that the stationary solution of Eq. (2.3) cannot be calculated in closed form; only approximate expressions are available [13].

In order to split the evolution operator  $e^{\tau L}$  into a product of exactly solvable parts, we partition the Fokker-Planck operator  $L$ , Eq. (2.3), into a leading (reference) contribution  $B$  and an anharmonic correction  $A$  reading

$$B = -v \partial_x + \gamma \partial_v (v + \gamma D \partial_v) \quad (2.4)$$

and

$$A = -\partial_x G(x). \tag{2.5}$$

As defined, the operator  $A$  describes the deterministic path of the system, and the operator  $B$  incorporates fluctuations away from this path. In what follows, by  $P_r(x, v, t|x_0, v_0)$  we shall mean the propagator of the reference process

$$P_r(x, v, t|x_0, v_0) = e^{tB} \delta(x-x_0) \delta(v-v_0), \tag{2.6}$$

whose explicit expression is given in the Appendix. Moreover, it is not difficult to show that

$$\exp[-t\partial_x G(x)]f(x) = J(x, t)f[H(x, t)], \tag{2.7}$$

where

$$J(x, t) \equiv \partial_x H(x, t) = G[H(x, t)]/G(x), \tag{2.8}$$

while the function  $H(x, t)$  is determined by the equation

$$H(x, t) = \exp[-tG(x)\partial_x]x. \tag{2.9}$$

The general solution of Eq. (2.9) is

$$H(x, t) = F^{-1}[F(x) - t], \quad F(x) = \int^x dy/G(y), \tag{2.10}$$

with  $F^{-1}$  being the inverse function, i.e.,  $F^{-1}[F(x)] = x$ . In the event that the integral in Eq. (2.10) is not doable analytically, the function  $H$  can be evaluated approximately by expanding the right-hand side of Eq. (2.9) in a Taylor series in  $t$ . To second order in  $t$  this gives

$$H(x, t) = x - tG(x) + \frac{1}{2}t^2G(x)G'(x) + O(t^3), \tag{2.11}$$

$$J(x, t) = \exp[-tG'(x) + \frac{1}{2}t^2G(x)G''(x)] + O(t^3),$$

where the prime denotes differentiation with respect to  $x$ . As shown in Ref. [7], approximations like Eq. (2.11) do not deteriorate the accuracy of Trotter-approximated propagators.

Now we are able to evaluate the short time propagator in the coordinate representation. Use of the above splitting together with the Trotter formula (1.5) yields the standard second-order approximation [3]

$$P_2(x, v, \tau|x_0, v_0) = J(x, \frac{1}{2}\tau)P_r[H(x, \frac{1}{2}\tau), v, \tau|H(x_0, -\frac{1}{2}\tau), v_0]. \tag{2.12}$$

In order to take higher-order corrections into account, we first have to evaluate the commutator  $C$ . The latter is easily determined in terms of Eqs. (1.11), (2.4), and (2.5) to give the operator

$$C = -\partial_x \mathcal{G}(x, v),$$

$$\mathcal{G}(x, v) = \frac{2}{3}G(x) + \frac{1}{72}\tau^2v[G(x)G''(x) - G'^2(x)], \tag{2.13}$$

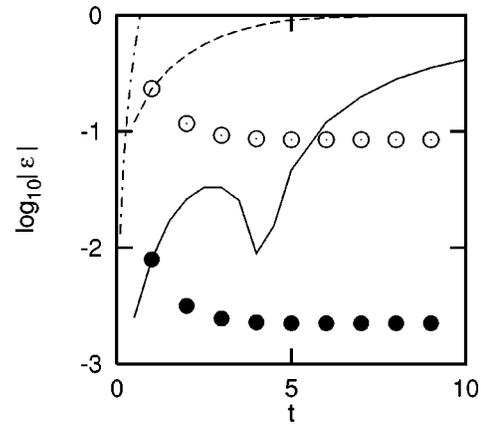


FIG. 1. Logarithm of the relative error  $\varepsilon = [(\text{approximate}) - (\text{exact})]/(\text{exact})$  in the second cumulant made by using Eqs. (2.12) (dashed line) and (2.15) (solid line) as single step propagators. Open and solid circles show the errors made by these propagators in the path integral evaluation, with  $\tau=1$ , of the same quantity. The dot-dashed line is for the fourth-order cumulant expansion of the single step propagator.

analogous to the drift operator  $A$  defined by Eq. (2.5). With this finding, we arrive at the fourth-order factorization

$$S_4(\tau) = e^{-\tau\partial_x G/6} e^{\tau B/2} e^{-\tau\partial_x \mathcal{G}} e^{\tau B/2} e^{-\tau\partial_x G/6}, \tag{2.14}$$

which appears as a product of two Trotter approximants, leaving us finally with

$$P_4(x, v, \tau|x_0, v_0) = J(x, \frac{1}{6}\tau) \int dy du P_r[H(x, \frac{1}{6}\tau), v, \frac{1}{2}\tau|\mathcal{H}(y, u, -\tau), u] \times P_r[y, u, \frac{1}{2}\tau|H(x_0, -\frac{1}{6}\tau), v_0]. \tag{2.15}$$

The function  $\mathcal{H}(x, v, t)$  involved in Eq. (2.15) is determined by Eqs. (2.9) and (2.10), if one replaces in these equations  $G(x)$  by  $\mathcal{G}(x, v)$ . It is thus seen that the new short time propagator, Eq. (2.15), requires an additional quadrature compared to the Trotter approximation, Eq. (2.12). On the other hand, the error accumulated in the  $N$  factors in the entire propagator, Eqs. (1.4) and (2.15), is of order  $N^{-4}$ ; consequently, the present propagator should allow larger time steps to be taken than the Trotter approximation for comparable accuracy. Thus the key question we shall address in numerical applications is the following: Does the increase in time step more than compensate for the added computational complexity?

Because closed-form analytic results are only available for a linear drift,

$$G(x) = -\omega x, \tag{2.16}$$

we tackle this problem for illustrating the power of the present technique. Figure 1 shows the relative error in the second cumulant,  $M_2(t) = \langle x^2(t) \rangle - \langle x(t) \rangle^2$ , made by using Eqs. (2.14) and (1.5) as *single step propagators*. The calculation is performed for  $D = \gamma = \omega = x_0 = v_0 = 1$ . Also shown is the error made by using the fourth-order cumulant expansion

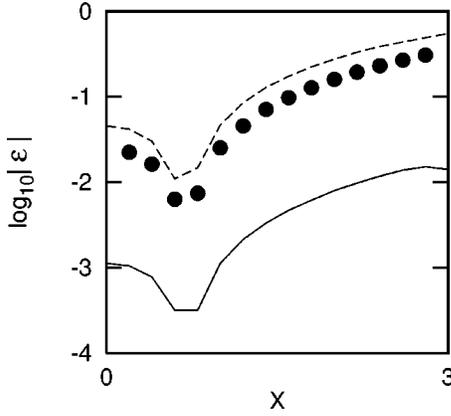


FIG. 2. Logarithm of the relative error in the path integral evaluation of the stationary solution, Eq. (2.17). The dashed and solid lines are, respectively, for Eqs. (2.12) and (2.15) with  $\tau=1$ . Circles are the result obtained after one folding of Eq. (2.15) with  $\tau=5$ .

sion of the propagator derived by one of us recently [12]. As anticipated, the error increases linearly with  $t$  in this case, and very soon grows out of the scale of the figure. The same is true to some degree for the Trotter splitting, whose error rapidly reaches 100%. In contrast, use of the fourth-order decomposition, Eq. (2.14), reduces the error over a broad range of  $t$  by nearly two orders of magnitude. This is especially pleasing since the properties of the free Brownian reference propagator employed in our calculation are very different from those of the Ornstein-Uhlenbeck process. The former describes the unrestricted diffusion spreading, while the latter has, for  $\omega>0$ , a nontrivial stationary solution. Hence one may conclude that the present technique shows promise for calculating not only short, but also intermediate time dynamics *analytically*.

However, the primary purpose we envision for Eq. (2.15) is an improved short time propagator for use in a path integral. Figure 1 also shows the errors made by Eqs. (2.14) and (1.5) in the path integral evaluation of the same quantity according to Eq. (1.4). It is seen that an acceptable precision of three significant digits is achieved in calculations with a relatively large time step  $\tau=1$  with the present fourth-order propagator. For comparison, the Trotter-approximated propagator provides an analogous accuracy just for  $\tau\lesssim 0.1$ , and thereby requires a computation that is five times as large. Analogous results for the cumulant expansion of the short time propagator are not presented in this case, as the latter fails grossly for  $\tau=1$ .

Next, Fig. 2 shows the relative errors in the path integral evaluation, with  $\tau=1$ , of the stationary solution  $P_e(x)$ ,

$$P_e(x) = \lim_{t \rightarrow \infty} \int_{-\infty}^{\infty} dv P(x, v, t). \quad (2.17)$$

The error made by the Trotter-approximated propagator is again two orders greater than that of Eq. (2.15). Thus the practical advantage offered by our formulation is that accurate results are obtainable with rather small values of  $N$  even though the net increment  $t$  is large. As seen in Fig. 2, a

precision of a few percent is achievable in the calculation of the stationary solution with a discretization as coarse as  $N=2$ , for  $\tau=5$ .

### III. KRAMERS EQUATION

As a second example, we consider the Kramers equation which is a special Fokker-Planck equation describing the Brownian motion in a potential  $U(x)$  [14]

$$\begin{aligned} \partial_t P(x, v, t) &= LP(x, v, t) \\ &\equiv [-v \partial_x + U'(x) \partial_v \\ &\quad + \gamma \partial_v (v + \beta^{-1} \partial_v)] P(x, v, t). \end{aligned} \quad (3.1)$$

Here  $\gamma$  denotes the friction coefficient, and  $\beta$  is the inverse temperature. The Kramers equation is commonly used in a number of problems of physics and chemistry, such as reaction kinetics, superionic conductors, nucleation, and Josephson tunneling junction [15]. As is the case with the colored noise problem, the diffusion matrix of Eq. (3.1) is singular. This equation, however, is more convenient for our purpose in the sense that it allows for a straightforward calculation of the stationary solution

$$P_e(x, v) = Z^{-1} \exp[-\beta v^2/2 - \beta U(x)], \quad (3.2)$$

with a partition function  $Z$ .

Proceeding along the same line as in Sec. II, we split the Fokker-Planck operator  $L$  defined by Eq. (3.1) into a linear reference part

$$B = -v \partial_x + \gamma \partial_v (v + \beta^{-1} \partial_v), \quad (3.3)$$

and the rest,

$$A = U'(x) \partial_v. \quad (3.4)$$

Insertion of these operators into the Trotter formula, Eq. (1.5), yields, in a straightforward way [3],

$$P_2(x, v, \tau | x_0, v_0) = P_r[x, v + \frac{1}{2} \tau U'(x), \tau | x_0, v_0 - \frac{1}{2} \tau U'(x_0)], \quad (3.5)$$

where the reference propagator  $P_r(x, v, t | x_0, v_0)$  is the same as in Eq. (2.12). It is given by Eqs. (A1), (A2), and (A3) with  $D = (\beta\gamma)^{-1}$  and  $\omega=0$ .

On the other hand, substituting Eqs. (3.3) and (3.4) into Eq. (1.11), we obtain

$$C = Q(x) \partial_v, \quad Q(x) = \frac{2}{3} U'(x) [1 - \frac{1}{24} \tau^2 U''(x)], \quad (3.6)$$

from which it follows that implementation of Eq. (1.9) is as simple in this case as that of the Trotter formula, Eq. (1.5). The resulting fourth-order propagator reads

$$\begin{aligned} P_4(x, v, \tau | x_0, v_0) &= \int dy du P_r[x, v + \frac{1}{6} \tau U'(x), \frac{1}{2} \tau | y, u \\ &\quad - \tau Q(y)] P_r[y, u, \frac{1}{2} \tau | x_0, v_0 - \frac{1}{6} \tau U'(x_0)]. \end{aligned} \quad (3.7)$$

In order to illustrate the power of the present scheme in treating nonlinear problems, we apply the various approxi-

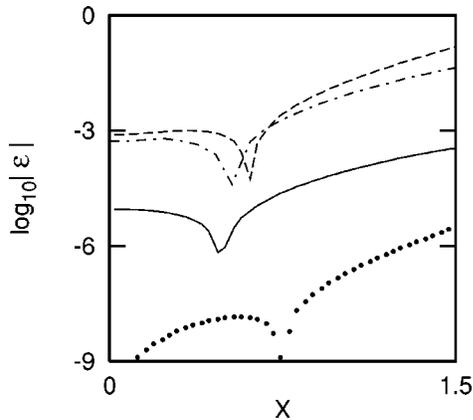


FIG. 3. Logarithm of the relative error in the path integral evaluation, with  $\tau=0.1$ , of the stationary solution of a Kramers model, Eqs. (3.1) and (3.8). Dashed line: Trotter formula, Eq. (3.5); dot-dashed line: fourth-order cumulant expansion; solid line: present fourth-order propagator, Eq. (3.7); dots: sixth-order propagator, Eq. (1.12).

mations discussed above for the short time propagator to the path integral evaluation of the stationary distribution  $P_e(x)$ . We take a symmetric potential of the form

$$U(x) = (x^2 + 1)^2, \quad (3.8)$$

and perform the calculation with  $\beta=1$  and  $\tau=0.1$ , for various different values of  $\gamma$ ,  $x_0$ , and  $v_0$ . The quadratures of Eqs. (1.4) and (3.7) 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 was developed in a previous paper [7]. The method employs the Stirling interpolation to readjust the distribution function every time step dynamically, with a mild increase in cost and with no loss of precision. Shown in Fig. 3 are results obtained for  $\gamma=5$  using the Trotter formula and the fourth-order factorization. Also shown are results obtained from the fourth-order cumulant expansion for the propagator [12]. As anticipated, the error made by the present propagation scheme is again much lower than those of the two other techniques. It is also seen that use of extrapolation (1.12) to remove  $1/N^4$  errors further increases the accuracy by nearly three orders of magnitude. For comparison, a precision of  $10^{-5}$  is attainable in calculations with the Trotter-approximated propagator just for  $\tau \leq 0.01$ . As to a precision of nine significant digits, the Trotter formula fails to provide it even though  $\tau=0.001$ .

It is also pleasing that the error made by using the present propagator turns out to be rather insensitive to  $\gamma$ ,  $x_0$ , and  $v_0$ . This is in drastic contrast to the cumulant expansion, whose accuracy deteriorates with increasing  $\gamma$ , and already for  $\gamma \sim 10$  the method fails to produce correct results. The reason is that the expansion for the second cumulant, which determines the width of the short time propagator, becomes negative for  $\gamma\tau > \frac{4}{3}$ . As a result, very short time steps are required for achieving the high-friction limit in this case.

#### IV. CONCLUSIONS

Our primary result is the demonstration that higher-order factorizations designed for solving classical and quantum problems are very effective when treating Fokker-Planck processes with singular diffusion matrices. In such a case, the various different operators involving higher-order derivatives may cancel so that the composite operator  $C$ , Eq. (1.11), is no more complicated than the drift term of the original Fokker-Planck operator. The resulting propagation scheme greatly reduces the error for a moderate number of time steps or requires, for comparable accuracy, considerably less computation than standard path integral methods now in use. Yet another attractive feature of the present scheme is that it is time reversible. Therefore, extrapolation methods for removing time slice errors can be employed to further improve its accuracy.

Finally, we would like to emphasize that we have not explicitly covered all possible cases to which our approach would apply. The method outlined above is also applicable to many other multidimensional Fokker-Planck processes whose operator can be partitioned into two exactly solvable parts such that the composite operator  $C$  possesses the exact solution. This happens to be so when the underlying stochastic system is of the type in Eqs. (2.3) or (3.1). However, this is not the generic case for any system with a noninvertible diffusion matrix. In particular, the method fails to treat efficiently models that are nonlinear both in  $x$  and in  $v$ . In addition, it may hardly be applied to multidimensional systems driven by multiplicative noise, as the latter cannot in general be converted to additive noise by a transformation of variables.

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#### APPENDIX

Although the exact solution for an arbitrary Ornstein-Uhlenbeck process can be found in a number of textbooks on stochastic processes (see, e.g., the book by Risken [15]), this solution is formal, and its application is far from straightforward in each particular case. The aim of this appendix is to explicitly solve the Fokker-Planck equation (2.3) for a linear drift coefficient, Eq. (2.16). Since the process is linear, the propagator is given by the two-variable Gaussian distribution

$$P(x, v, t | x_0, v_0) = \frac{1}{2\pi\sqrt{M(t)}} \exp \left\{ -\frac{M_{vv}(t)}{2M(t)} [x - M_x(t)]^2 + \frac{M_{xv}(t)}{M(t)} [x - M_x(t)][v - M_v(t)] - \frac{M_{xx}(t)}{2M(t)} [v - M_v(t)]^2 \right\}, \quad (A1)$$

with mean values

$$M_x(t) = x_0 e^{-\omega t} - v_0 (e^{-\omega t} - e^{-\gamma t}) / (\omega - \gamma), \quad (\text{A2})$$

$$M_v(t) = v_0 e^{-\gamma t},$$

$$M_{xv}(t) = \frac{\gamma^2 D}{\omega - \gamma} \left\{ \frac{1}{\gamma} (1 - e^{-2\gamma t}) - \frac{2}{\omega + \gamma} [1 - e^{-(\omega + \gamma)t}] \right\}, \quad (\text{A3})$$

and variances

$$M_{xx}(t) = \frac{\gamma^2 D}{(\omega - \gamma)^2} \left\{ \frac{1}{\omega} (1 - e^{-2\omega t}) + \frac{1}{\gamma} (1 - e^{-2\gamma t}) - \frac{4}{\omega + \gamma} [1 - e^{-(\omega + \gamma)t}] \right\},$$

$$M_{vv}(t) = \gamma D (1 - e^{-2\gamma t}).$$

In the above,  $M(t) = M_{xx}(t)M_{vv}(t) - M_{xv}^2(t)$ . Finally, the expression for the reference propagator  $P_r(x, v, t | x_0, v_0)$  follows from the present solution for  $\omega \rightarrow 0$ .

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