Time mapping in power series expansions for the time evolution operator

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Two formally equivalent methods for systematically evaluating either the propagator or the average of dynamical variables are developed by expanding these quantities in a power series in a given function $\tau(t)$. The expansion coefficients are analytically determined by recursion relations. The methods are an extension of our power series expansion formalism [Phys. Rev. Lett. **75**, 4342 (1995)] to a general Fokker-Planck-Schrödinger process. The role of the time transformation in accelerating the series convergence is emphasized and the generalization to an arbitrary conformal time mapping $\tau(t)$ is presented. An appropriate truncation scheme is suggested to eliminate the openness of the series representations. We also develop a regular procedure to minimize the truncation error. The formalism thus constructed provides a basis for an efficient error controlled treatment of simple or complex systems with any number of degrees of freedom. The application to a well-known problem of the decay of an unstable state driven by exponentially correlated Gaussian noise shows that an accurate description for arbitrarily large t is attained with a few terms of the present expansions and their utility is rather insensitive with respect to the noise strength. This is in contrast to the various available approximate solutions of the problem that are all asymptotic in the noise strength. [S1063-651X(97)12102-X]

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I. INTRODUCTION

There is a wide class of phenomena in physics, chemistry, and biology whose dynamics and statistical mechanics can properly be described in terms of Fokker-Planck, Bloch, and Schrödinger equations [1,2]. These equations, which will be subsumed under the name Fokker-Planck equation, typically have the form (a summation over repeated indices is always implied, if not stated otherwise)

$$\partial_t P(\mathbf{x},t) = cLP(\mathbf{x},t) \equiv c\left[\frac{1}{2}\partial_{ij}^2 D_{ij}(\mathbf{x}) - \partial_i G_i(\mathbf{x}) - V(\mathbf{x})\right] P(\mathbf{x},t) \tag{1}$$

and are to be solved with some initial condition $P(\mathbf{x},0)$. Here L is the Fokker-Planck operator defined by Eq. (1), $\mathbf{x}^T=(x_1,\ldots,x_n)$, and the number c defines the problem under study: for complex $c=\imath$ Eq. (1) is a Schrödinger equation and for $c=1$ it is a Fokker-Planck or Bloch-type equation. Since c can always be absorbed into L, we set $c=1$ from here on. General solutions of Eq. (1) can be derived in many different ways, e.g., by using path-integral methods or eigenmode expansion [1,2]; but the solutions thus obtained are formal. There are very few models that can be solved exactly with presently known mathematical techniques. This situation gives rise to many stimulating opportunities for the development of approximate procedures to analyze such equations numerically. Widely used procedures rest on basis set expansion [2–7], path integrals [3,8–14], iterative time-dependent propagation schemes [3,15–20], and moment expansion [21–23]. Numerical schemes can, in principle, provide very accurate results with intensive computational efforts. Their utility, however, is strongly limited by the storage requirements and execution time that grow exponentially with the dimensionality of the problem under study. Various approximate methods could also be very efficient in analytically treating Eq. (1), provided that their assumptions are satisfied. Some of these methods rely on the specific nature of the equation and almost all of them involve approximations that limit their applicability to certain favorable regimes of parameter space and/or initial conditions. The reader is referred to various quasiharmonic and quasiadiabatic approximations [12,24–26], as well as to perturbation techniques based on the generalized Trotter formula [27–32], Dyson series expansion [33,34], semiclassical approximation [35,36], and Taylor series representation in t [37–40] (see also a collection of references in Ref. [39]). The latter method is particularly efficient from the computational point of view. Being formally exact, a Taylor series representation of the time evolution operator, in contrast to those obtained in terms of path-integral methods and eigenmode expansion, provides a very natural basis for the *systematic evaluation* of the fundamental solution (propagator) of Eq. (1), satisfying the initial condition

$$P(\mathbf{x},t=0|\mathbf{y}) = \delta(\mathbf{x}-\mathbf{y}) \tag{2}$$

in a *straightforward, analytical* way.

In the following, by a Taylor series representation of the propagator we will mean any representation of the form

$$P(\mathbf{x},t|\mathbf{y}) = K(\mathbf{x},t|\mathbf{y})Z(S),$$
$$S = t^m P_m(\mathbf{x},\mathbf{y}), \tag{3}$$

where $K(\mathbf{x},t|\mathbf{y})$ and $Z(S)$ are given functions. The existing approaches are not generally different from each other, but rather their choices for these functions [37–40]. Depending on the definition of K and Z, different recursion relations for

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the expansion coefficients P_m are derived by inserting Eq. (3) into the original equation and equating like powers in t. The recursion relations are simple enough to permit the analytic evaluation of the expansion coefficients for any number of degrees of freedom in many situations of practical interest. Analogous results are also obtainable by other means [35,41,42]. But the reader can readily verify that the derivation outlined above is considerably simpler and shows more systematically how terms of arbitrary order can be determined. One also notes that many other available series representations for the propagator though systematic, are purely formal and therefore no more simple to implement than the original Fokker-Planck equation [33,34,36].

Although the Taylor series expansion method can be used to solve general Fokker-Planck equations [39], its convergence has not been theoretically proven. However, the calculations, performed on model systems using Eq. (3) with different functions K and Z, show that the utility of the method is in general restricted to short times [37,38,43–45]. The method is actually accurate in this limit if one truncates the series at high enough order. With increasing t the number of terms necessary for obtaining accurate results grows very rapidly, and beyond some $t_{\max}$ that is usually noticeably smaller than unity, the expansion fails to converge with a finite number of terms involved in the series. Even though any reasonable number of the expansion coefficients P_m are obtainable analytically, e.g., by using a computer algebra manipulator, it is practically impossible with this technique to approximately evaluate intermediate-time dynamics, to say nothing of dynamics in the whole time domain [37,45]. The reason is that a finite-order truncation of the series (3) at $m=M$, as t goes to infinity, also tends to plus or minus infinity depending on the sign of $P_M(\mathbf{x},\mathbf{y})$. This is the case regardless of the specific form of the Fokker-Planck operator and initial conditions.

In a recent series of papers [43–45], we have presented an alternative power series expansion formalism that is free of the above drawback. Its key points are representing the full propagator as a product of the harmonic-oscillator propagator with the configuration function and expanding the exponent of the configuration function in a power series in a given function $\tau(t)$ in place of t. The explicit form of the function $\tau(t)$ introduced in Refs. [43–45] reads

$$\tau=\frac{1}{\omega}(1-e^{-\omega t}). \tag{4}$$

This particular time dependence has been chosen as it is associated with the width of the reference harmonic-oscillator propagator and so it is hoped to give a reasonable time scale in a general case. From a computational point of view, the most appealing feature of this approach is perhaps that the fictitious time τ maps the singular point $t=\infty$ to finite $\tau=1/\omega$. In addition, the frequency ω, which is a free parameter, can be chosen such that the convergence of the corresponding series in τ is as fast as possible. Numerical applications to various physical models show this formalism to be a dramatic improvement over the existing Taylor series expansions of the propagator, Eq. (3), in that it converges much better over a much broader range of t [43–45]. However, the results thus obtained are not exhaustive with respect to methodology. Their utility is generally restricted to equations with constant and invertible diffusion matrix and, what is also important, to this particular dependence τ of t, Eq. (4). Moreover, the convergence rate is found to be very sensitive to the choice of the free parameter ω involved in the expansion, but we have failed to develop a rather rigorous and general method for its determination.

In this paper, two essentially analytic techniques for generating series representations, one for the propagator and another one for the average of a dynamical variable associated with $P(\mathbf{x},t)$, are presented. These are an extension of our power series expansion formalism [43–45] to a general Fokker-Planck process, Eq. (1), as well as to an arbitrary dependence τ of t. Our aim is to provide a systematic, error controlled strategy for grouping the terms in the Taylor series (3) so that the terms of the rearranged series decrease much faster. Clearly, this strategy permits the efficient extrapolation of the behavior of the series to its eventual sum for as large as a time interval as possible. A slowly converging power series such as in Eq. (3) can always be cast into the form

$$S=\tau^m W_m(\mathbf{x},\mathbf{y}), \tag{5}$$

where τ is an arbitrary conformal time transformation $\tau(t)$ satisfying the condition $\tau(0)=0$. Certainly, such a representation of the propagator is actually equivalent to its original Taylor series representation. The only reward for making the problem more complicated is that we can thus apply all the machinery for sum acceleration to the new series Eq. (5). In particular, experience shows that the Taylor series in (3) is usually an alternating one in a wide range of $\mathbf{x}$ and $\mathbf{y}$. Therefore, one may expect that a generalized Euler transformation of the form

$$\tau=\frac{t}{1+\omega t}, \tag{6}$$

which is known to be ''the old reliable'' of sum acceleration algorithms for alternating series, would be especially useful in such a case. The advantage of this transformation is that when applied to almost any alternating series that is converging or diverging algebraically, it yields a new series that converges exponentially fast.

The general developments are given in Secs. II and III for the propagator and for the average of dynamical variables, respectively. Different schemes for truncating the series representations are discussed in Sec. IV. Numerical calculations for test systems are presented in Sec. V. Sections VI ends the paper with an outlook.

II. POWER SERIES EXPANSION FOR THE PROPAGATOR

Following the underlying idea of the present paper, outlined in the Introduction, we first replace in Eq. (1) the time derivative ∂_t by that over τ

$$\partial_t=\frac{d\tau}{dt}\partial_\tau, \tag{7}$$

where a series expansion in τ for $d\tau/dt$ is assumed to exist,

$$\frac{d\tau}{dt}=1+\xi_m\tau^m, \quad m\geqslant 1. \tag{8}$$

In this expansion we have set, without loss of generality, $\xi_0=1$, in order to provide the equality $\tau=t$ for $\xi_i=0$ $(i\geqslant 1)$. The inverse of the diffusion matrix, $D^{ij}=(D_{ij})^{-1}$, is also assumed to exist, thus permitting us to interpret it as the metric of a Riemannian manifold spanned by the variables x_i. Then, Eq. (1) can exactly be solved by expanding the exponent of the propagator in powers of $\tau(t)$

$$P(\mathbf{x},t|\mathbf{y})=[(2\pi\tau)^n D(\mathbf{x})]^{-1/2}\exp[\tau^{m-1}W_m(\mathbf{x},\mathbf{y})], \quad m\geqslant 0, \tag{9}$$

with $D(\mathbf{x})$ being the determinant $D(\mathbf{x})=\det[D_{ij}(\mathbf{x})]$. It is a simple matter to check that the ansatz (9) reduces the original problem to the following hierarchy of first-order coupled differential equations for the expansion coefficients $\{W_m(\mathbf{x},\mathbf{y})\}$:

$$D_{ij}(\partial_i W_0)(\partial_j W_m)-(m-1)W_m-V_m=0. \tag{10}$$

In Eq. (10) the summation rule for m is not implied, while the inhomogeneity V_m is determined in terms of lower-order terms $(W_{-1}=\xi_{-1}=0)$,

$$\begin{aligned}V_m=&\frac{1}{2}D_{ij}(\partial_i W_0)(\partial_j W_0)\delta_{m,0}+(\partial_i h_i+\Gamma^i_{ij}h_j+V)\delta_{m,2}\\&+\left(h_i+\frac{1}{2}D_{kj}\Gamma^i_{kj}\right)\partial_i W_{m-1}-\frac{n}{2}\xi_{m-1}\\&+\sum_{i=0}^{m-1}(i-1)\xi_{m-i}W_i\\&-\frac{1}{2}D_{ij}\left[\partial^2_{ij}W_{m-1}+\sum_{k=1}^{m-1}(\partial_i W_k)(\partial_j W_{m-k})\right],\end{aligned} \tag{11}$$

where Γ^k_{ij} stands for a Christoffel symbol

$$\Gamma^k_{ij}=\frac{1}{2}D_{kr}(\partial_i D^{rj}+\partial_j D^{ri}-\partial_r D^{ij}) \tag{12}$$

and h_i for

$$h_i=G_i+\frac{1}{2}D_{kj}\Gamma^i_{kj}. \tag{13}$$

It should be noted that at this stage the boundary conditions for Eq. (1) and thus the ones for Eq. (10) are left completely unspecified. For simplicity 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 expansion coefficients.

For $m=0$ the equation reads

$$D_{ij}(\partial_i W_0)(\partial_j W_0)+2W_0=0. \tag{14}$$

To the best of our knowledge, there are no general solutions of this equation for curved manifolds other than a formal expansion in terms of $\eta_i=x_i-y_i$ derived by representing D^{ij} in a ''product'' form

$$D^{ij}=g^{ik}g^{jk}. \tag{15}$$

Due to the symmetry and reality of D^{ij} the real and symmetric matrix g^{ij} always exists. It is generally defined as

$$g^{ij}=\varphi^{(k)}_i\lambda^{1/2}_k\varphi^{(k)}_j, \tag{16}$$

with $\{\varphi^{(k)}_i\}$ and $\lambda_k(i,k=1,\ldots,n)$ being, respectively, the eigenvectors and eigenvalues of D^{ij}. If one expands $W_0(\mathbf{x},\mathbf{y})$ in powers of η_i, the formal solution to Eq. (14) reads [39]

$$W_0(\mathbf{x},\mathbf{y})=-\frac{1}{2}|(\boldsymbol{\eta}\cdot\nabla)^{k-1}\mathbf{g}^{-1}\boldsymbol{\eta}/k!|^2, \quad k\geqslant 1. \tag{17}$$

In the series (17) ∇ acts on $\mathbf{g}^{-1}$ only, and the derivatives of $\mathbf{g}^{-1}$ are evaluated at $\mathbf{x}=\mathbf{y}$. The first few terms of this expansion can be determined explicitly

$$\begin{aligned}W_0(\mathbf{x},\mathbf{y})=&-\frac{1}{2}D^{ij}\eta_i\eta_j-\frac{1}{2}\{D^{r\cdot}\Gamma^{r}_{\cdot\cdot}\}_{ijk}\eta_i\eta_j\eta_k\\&+\frac{1}{24}\{D^{ps}\Gamma^{p}_{\cdot\cdot}\Gamma^{s}_{\cdot\cdot}-2\partial^2_{\cdot\cdot}D^{\cdot\cdot}\}_{ijkr}\eta_i\eta_j\eta_k\eta_r\\&+\cdots,\end{aligned} \tag{18}$$

where the curly brackets denote complete symmetrization, i.e.,

$$\{D^{r\cdot}\Gamma^{r}_{\cdot\cdot}\}_{ijk}=\frac{1}{3}(D^{ri}\Gamma^r_{jk}+D^{rj}\Gamma^r_{ik}+D^{rk}\Gamma^r_{ij}). \tag{19}$$

The rest of the equations in the hierarchy (10) are linear with respect to W_m and readily solved in closed form to yield [39]

$$\begin{aligned}W_m(\mathbf{x},\mathbf{y})=&\frac{1}{2}[-W_0(\mathbf{x},\mathbf{y})]^{(1-m)/2}\int_{\mathbf{y}}^{\mathbf{x}}dz_i[\partial_i W_0(\mathbf{z},\mathbf{y})]\\&\times[-W_0(\mathbf{z},\mathbf{y})]^{(m-3)/2}V_m(\mathbf{z},\mathbf{y})\\=&\frac{1}{2}[-W_0(\mathbf{x},\mathbf{y})]^{(1-m)/2}\int_0^1 du\,\eta_i[\partial_i W_0(\mathbf{q},\mathbf{y})]\\&\times[-W_0(\mathbf{q},\mathbf{y})]^{(m-3)/2}V_m(\mathbf{q},\mathbf{y}),\end{aligned} \tag{20}$$

where $\mathbf{q}=\mathbf{y}+u(\mathbf{x}-\mathbf{y})$. One notes, however, that with Eq. (17) it is a far from simple task to evaluate even the first expansion coefficients W_1. The calculations very rapidly become arduous. A closed-form solution for W_0 is therefore particularly desirable. We suggest that with this technique each problem should be studied separately in curved manifolds.

In flat spaces the curvature tensor associated with D^{ij} vanishes, which considerably simplifies calculating W_m. In this case, the matrix g^{ij} must satisfy the equation

$$\partial_k g^{ij} = \Gamma^r_{ik} g^{rj}, \tag{21}$$

whose formal solution reads

$$g^{ij}(\mathbf{x}) = \exp\left[\int_{\mathbf{y}}^{\mathbf{x}} dz_k \Gamma^r_{ik}(\mathbf{z}) \right] g^{rj}(\mathbf{y}). \tag{22}$$

Moreover, there exists a change of variables determined by

$$Q_i(\mathbf{x}) = \int^{\mathbf{x}} dz_j g^{ji}(\mathbf{z}), \tag{23}$$

such that admits a closed-form solution to Eq. (17),

$$W_0(\mathbf{x},\mathbf{y}) = -\frac{1}{2}|\mathbf{Q}(\mathbf{x}) - \mathbf{Q}(\mathbf{y})|^2. \tag{24}$$

With Eq. (24) the first few terms of the present expansion are easily determined explicitly to give

$$W_1 = \frac{1}{2}\xi_1 W_0 + \int_{\mathbf{y}}^{\mathbf{x}} dz_i D^{ij}(\mathbf{z}) h_j(\mathbf{z}), \tag{25}$$

$$W_2 = -\int_0^1 du\ V_2(\mathbf{Z}), \tag{26}$$

$$W_3 = -\frac{1}{2}\xi_1 W_2 + \frac{n}{4}\xi_2 + \frac{1}{4}\xi_3 W_0 - \frac{1}{2}\int_0^1 du\ u(1-u) \times [D_{ij}(\partial^2_{ij} - \Gamma^k_{ij}\partial_k) V_2]|_{\mathbf{Z}}. \tag{27}$$

Here V_2 is a known function

$$V_2 = V + \frac{1}{2}(\partial_i h_i + \Gamma^j_{ij} h_i + D^{ij} h_i h_j) + \left(\frac{1}{4}\xi_1^2 - \xi_2\right) W_0 - \frac{n}{4}\xi_1, \tag{28}$$

$\mathbf{Z} = \mathbf{Q}^{-1}[\mathbf{Q}(\mathbf{y}) + u(\mathbf{Q}(\mathbf{x}) - \mathbf{Q}(\mathbf{y}))]$, and $\mathbf{Q}^{-1}$ means the inverse transformation from $\mathbf{Q}$ to $\mathbf{x}$, i.e. $\mathbf{Q}^{-1}[\mathbf{Q}(\mathbf{x})] = \mathbf{x}$.

It is a simple matter to verify that the various different Taylor series representations available for the propagator [37,39,41,42] follow from the above results in a very natural way for $\tau = t$. We also emphasize that the evaluation of the expansion coefficients W_m requires no additional computational effort compared to those of the Taylor series expansions. The connection of the present results with the harmonic-oscillator representation of the propagator developed in our earlier papers [43,44] is not so easily established. Although all the series representations are formally equivalent, there can be practical advantages to choosing one over the others. When studying complex anharmonic systems, the present expansion is the more natural choice. One of the advantages in the use of this expansion, apart from its generality, is that it is expected to produce a more rapid convergence due to an appropriately chosen time transformation. Finally, we note that the present results are easily generalized to the case of time-dependent operators [44].

Two disadvantages of this method, which are also inherent to almost all the other series representations of the propagator, are as follows. The method is efficient if and only if the coefficients of the Fokker-Planck equation V, G_i, and D_{ij} are simple enough so that the various integrals in Eq. (20) are doable analytically. Otherwise numerical quadratures are required. The latter restricts considerably the utility of the series representation. Another disadvantage is that the present results are applicable to the Fokker-Planck equation whose diffusion matrix is invertible. Its invertibility, however, is not a generic case. There is a wide class of equations with noninvertible (singular) diffusion matrices that play a central role in many scientific areas, most notably in chemical kinetics, theory of nucleation, and nonlinear optics, to name only a few [2]. Below we present an alternative power series representation free of these two drawbacks.

III. POWER SERIES EXPANSION FOR THE AVERAGE OF DYNAMICAL VARIABLES

It is known that the time evolution of true Fokker-Planck systems, Eq. (1) with $c = 1$ and $V(\mathbf{x}) = 0$, can be studied in a formally equivalent way by following either the distribution function or the average of the dynamical variable of interest. The latter is defined by

$$\langle a(t) \rangle = \int d\mathbf{x}\ P(\mathbf{x},t) a(\mathbf{x}). \tag{29}$$

It is a simple matter to show that Eq. (29) can be cast into the form

$$\langle a(t) \rangle = \int d\mathbf{x}\ P(\mathbf{x},0) A(\mathbf{x},t), \tag{30}$$

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

$$\partial_t A(\mathbf{x},t) = L^+ A(\mathbf{x},t) \equiv \left[\frac{1}{2} D_{ij}(\mathbf{x}) \partial^2_{ij} + G_i(\mathbf{x}) \partial_i\right] A(\mathbf{x},t) \tag{31}$$

supplemented by the initial condition $A(\mathbf{x},0) = a(\mathbf{x})$. Our aim is to develop a power series representation for $\langle a(t) \rangle$ that is valid and easily implemented irrespective of the particular form of the Fokker-Planck operator. A straightforward way for achieving this is to use the ansatz

$$\langle a(t) \rangle = a_m \tau^m, \quad a_m = \int d\mathbf{x}\ P(\mathbf{x},0) A_m(\mathbf{x}), \quad m \geq 0, \tag{32}$$

corresponding to the expansion

$$A(\mathbf{x},t) = A_m(\mathbf{x}) \tau^m, \quad m \geq 0. \tag{33}$$

The associated recursion relation reads

$$m A_m(\mathbf{x}) = L^+ A_{m-1}(\mathbf{x}) - \sum_{i=1}^{m-1} i \xi_{m-i} A_i(\mathbf{x}), \tag{34}$$

where the summation rule for m is not implied and L^+ is the backward Fokker-Planck operator defined by Eq. (31). As seen from the above equation, the expansion coefficients of the series (33) are readily determined recursively in terms of the Fokker-Planck coefficients and their derivatives, starting with $A_0(\mathbf{x}) = a(\mathbf{x})$ ($A_m = 0$ for $m < 0$). In contrast to Eqs. (9) and (10), the calculations are rather trivial *regardless* of the

specific dependence of V, G_i, and D_{ij} on $\mathbf{x}$. What is also pleasing is that the method outlined above is applicable, whether the diffusion matrix is invertible or singular.

We believe this method will provide the necessary foundation for systematically treating a variety of physically meaningful models, such as a Kramers equation and a colored-noise problem [2,32], that are difficult to treat by other means. For example, it is hoped to greatly help visualization of various correlation functions of the form

$$\langle a(t)b(0)\rangle = \int d\mathbf{x}\, d\mathbf{y}\; a(\mathbf{x})P(\mathbf{x},t|\mathbf{y})b(\mathbf{y}), \tag{35}$$

which play an important role in the theory of stochastic processes [46]. One also notes that the method can be modified to cover truly nonlinear Fokker-Planck equations whose coefficients exhibit a functional dependence on the distribution function $P(\mathbf{x},t)$ [45]. 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 presents a sufficiently difficult and often impossible task.

Before closing this section two remarks are in order. First, we note that the corresponding series representation for the distribution function, which is equivalent to Eq. (33) and formally applicable to any Fokker-Planck operator, reads

$$P(\mathbf{x},t) = B_m(\mathbf{x})\tau^m, \quad m \geqslant 0, \tag{36}$$

where the expansion coefficients $B_m(\mathbf{x})$ are generated by

$$mB_m(\mathbf{x}) = LB_{m-1}(\mathbf{x}) - \sum_{i=1}^{m-1} i\xi_{m-i}B_i(\mathbf{x}), \tag{37}$$

with $B_0(\mathbf{x}) = P(\mathbf{x},0)$. One must be cautious, however, on the use of this expansion, as a finite truncation of the series in Eq. (37) does not possess an important property that is shared by the true probability distribution, namely,

$$P(\mathbf{x},t) \geqslant 0 \quad \forall \mathbf{x},t. \tag{38}$$

Of course, the inequality (38) has no sense in real-time quantum-mechanical calculations, Eq. (1) with $c = \imath$, in which case $P(\mathbf{x},t)$ is a complex function, but it generally holds for a diffusion process ($c = 1$).

Another remark concerns an exponential power series representation of the form

$$P(\mathbf{x},t) = \exp[C_m(\mathbf{x})\tau^m], \quad m \geqslant 0, \tag{39}$$

whose coefficients are determined by

$$\begin{aligned} mC_m = {} & \left(\frac{1}{2}\partial_{ij}^2 D_{ij} - \partial_i G_i - V\right)\delta_{m,1} + [(\partial_i D_{ij}) - G_j]\partial_j C_{m-1} \\ & - \sum_{i=1}^{m-1} i\xi_{m-i}C_i + \frac{1}{2}D_{ij} \\ & \times \left[\partial_{ij}^2 C_{m-1} + \sum_{k=0}^{m-1} (\partial_i C_k)(\partial_j C_{m-1-k})\right] \end{aligned} \tag{40}$$

with $C_0(\mathbf{x}) = \ln P(\mathbf{x},0)$. One might think that the above expansion could be successfully employed for overcoming the negative sign problem. But our calculations performed with Eqs. (39) and (40) for model systems show that the utility of these equations is rather restrictive with respect to the initial conditions and the Fokker-Planck coefficients. We have found, in particular, that an accurate description for the whole time domain is obtainable with this technique if and only if the width of the initial distribution $P(\mathbf{x},0)$ is sufficiently large, while the coefficients V, G_i, and D_{ij} are sufficiently smooth functions of $\mathbf{x}$. Otherwise it works no better than the standard Taylor series expansion, being useful for short times only.

IV. TRUNCATION SCHEMES

Generally, series representations are not closed. There are two factors that render their recursion relations open. First, the solution of the Fokker-Planck equation cannot, in general, be expanded in terms of limited order polynomials in τ (or t). A truncation scheme must therefore be employed to eliminate this openness. A trivial procedure is to neglect all terms of higher order than some $m = M$. The approximate solution thus obtained (in the following we will use the subscript M in order to distinguish it from the exact solution) is presumably correct in the short-to intermediate time regime. But it is not necessarily valid in the limit $t \to \infty$. So a fruitful way of overcoming the openness is to employ a truncation scheme based on the stationary solution of the problem under study provided that is known exactly. One notes that this concept is meaningful only for a true Fokker-Planck process, Eq. (1) with $c = 1$ and $V(\mathbf{x}) = 0$, in which case it is determined by

$$P_{\mathrm{st}}(\mathbf{x}) = \lim_{t\to\infty} P(\mathbf{x},t|\mathbf{y}) = \mathcal{P}_0(\mathbf{x}). \tag{41}$$

Here $\mathcal{P}_0(\mathbf{x})$ is the eigenfunction of the forward Fokker-Planck operator corresponding to the lowest eigenvalue $\lambda_0 = 0$, $L\mathcal{P}_0 = 0$. It is also worthwhile noticing that an explicit integral expression for the stationary distribution in terms of the drift G_i and diffusion D_{ij} coefficients exists if and only if these coefficients satisfy the so-called potential conditions [2].

In order to introduce P_{st} into the series (9), we first write the propagator in the form

$$P(\mathbf{x},t|\mathbf{y}) = F(\mathbf{x},\mathbf{y};t)P_M(\mathbf{x},t|\mathbf{y}), \tag{42}$$

where F is a correction function defined by Eq. (42). The above equation is actually exact for any truncation number M; the only advantage of breaking up the propagator according to Eq. (42) is that we can thus use on the right-hand side of Eq. (42) instead of the exact correction function its approximation, which needs be accurate only in the long-time limit. In constructing such an approximation it is sufficient to satisfy the conditions

$$\begin{aligned} & \lim_{t\to\infty} F(\mathbf{x},\mathbf{y};t) = P_{\mathrm{st}}(\mathbf{x})/P_M(\mathbf{x},t\to\infty|\mathbf{y}), \\ & \lim_{t\to 0} F(\mathbf{x},\mathbf{y};t) = 1 + O(\tau^K), \end{aligned} \tag{43}$$

with $K \geqslant M-1$. The latter inequality follows from the fact that the error due to truncating the series in Eq. (9) at $m=M$ is of the order of τ^{M-1} (see below). A simple choice for F reads

$$F_M(\mathbf{x},\mathbf{y};t)=\exp\left\{\left(\frac{\tau}{\tau_\infty}\right)^{M-1}\ln[P_{\rm st}(\mathbf{x})/P_M(\mathbf{x},t\to\infty|\mathbf{y})]\right\}, \tag{44}$$

where $\tau_\infty=\tau(t\to\infty)$. The global approximation so constructed,

$$P_M^g(\mathbf{x},t|\mathbf{y})=F_M(\mathbf{x},\mathbf{y};t)P_M(\mathbf{x},t|\mathbf{y}), \tag{45}$$

is obviously exact for $t=0$ and $t=\infty$. One can thus expect that it would be reasonably accurate in the intermediate-time domain as well. For completeness we also present an analogous global approximation for $A(\mathbf{x},t)$. It reads

$$A_M^g(\mathbf{x},t)=A_M(\mathbf{x},t)+\left(\frac{\tau}{\tau_\infty}\right)^M[A_{st}-A_M(\mathbf{x},t\to\infty)], \tag{46}$$

where

$$A_{\rm st}=\int d\mathbf{x}\ P_{\rm st}(\mathbf{x})a(\mathbf{x}). \tag{47}$$

Clearly, the same technique can be used in order to properly incorporate a known time-dependent long-time limit solution of the problem of interest, whatever the Fokker-Planck operator is.

The other openness comes from the series representation of the derivative $d\tau/dt$, Eq. (7). A straightforward way of removing this openness is either to truncate the series (7) at $m=M-1$ or to use a function $\tau(t)$ such that its time derivative is expanded in terms of a limited order polynomial in τ. In both cases, the expansion coefficients ξ_i are considered as free parameters and the problem of importance is to determine them so that the approximate solution (P_M or A_M) is correct over as large as a time interval as possible. A simple, intuitive approach to the determination of the free parameters is to fix them from the sole knowledge of some relevant values of the system under study. Usually the available information is the normalization condition

$$N\equiv\int d\mathbf{x}\ \theta(\mathbf{x},t)=1, \tag{48}$$

where $\theta=|\Psi(\mathbf{x},t)|^2$ for the Schrödinger equation and $\theta=P(\mathbf{x},t|\mathbf{y})$ for the true Fokker-Planck equation. With the approximate propagator P_M, Eq. (48) constitutes an integral equation for the unknown parameters ξ_i as functions of time. Although the results in selected examples appear to be accurate [44], such a choice of ξ_i would seem to lack a sound theoretical basis. Besides, for cases with more than one free parameter the solution of Eq. (48) is not unique. What is also important is that this method is not generally suitable for the power series expansion for the average, Eq. (33), as the corresponding series expansion for the propagator, Eq. (36), automatically satisfies the normalization condition, no matter what t, M, and ξ_i are. The same is true, in one sense or another, for the other methods we have already discussed in our previous articles [43–45]. Some of these methods are very difficult to implement and almost all of them rely on the specific properties of the considered equation limiting the applicability of the methods to certain kind of situations.

In the reminder of this section, a general error controlled method is outlined that is rather simple, but also rigorous and allows the efficient, self-consistent treatment of the present series expansions without resorting to any external observations. To be specific, we restrict our considerations to the function

$$\tau=\frac{1-e^{-\mu t}}{\omega+(\mu-\omega)e^{-\mu t}}. \tag{49}$$

The corresponding coefficients ξ_i are given by

$$\xi_1=\mu-2\omega,\quad \xi_2=\omega(\omega-\mu),\quad \xi_i=0,\quad i>2.$$

One can easily check that for $\mu=\omega$ this time transformation reduces to that already used in our earlier papers [43–45], Eq. (4), while for $\mu=0$ it gives the generalized Euler transformation (6). Clearly, the best way of treating a power series expansion is to study its convergence properties as a function of free parameters. Unfortunately, establishing general convergence properties for the series representations developed in Secs. II and III is a quite difficult task. The expansion coefficients of these representations are determined recursively and therefore cannot be expressed in closed form. Since, however, the error introduced in $P_M(\mathbf{x},t|\mathbf{y})$ and $A_M(\mathbf{x},t)$ due to the series truncation is a function of the free parameters ξ_i, a rigorous way for their determination is to minimize this error in one or another sense. Let the error operator be $\rho=\partial_t-L$. When applied to the approximate propagator P_M, it leads in a straightforward way to the following expression for the error:

$$\begin{aligned}\varepsilon_P=\Big\{&\xi_2(M-1)W_M\tau^M\\&+[D_{ij}(\partial_iW_0)(\partial_jW_{M+1})-MW_{M+1}]\tau^{M-1}\\&-\frac{1}{2}D_{ij}\sum_{k=2}^{M}\sum_{r=M+2-k}^{M}(\partial_iW_k)(\partial_jW_r)\tau^{k+r-2}\Big\}P_M.\end{aligned} \tag{50}$$

A good approximation for the propagator can then be obtained by minimizing the error functional

$$I_P(\omega,\mu)=\int_0^T dt\int d\mathbf{x}[\varepsilon_P(\mathbf{x},t)]^*[\varepsilon_P(\mathbf{x},t)] \tag{51}$$

with respect to ω and μ. Here the asterisk denotes the complex conjugate, while $[0,T]$ is the interval in which an accurate description is required. We note that the optimal values of ω and μ so obtained turn out to be rather insensitive with respect to T. On the other hand, as the truncation error $\varepsilon_P(\mathbf{x},t)$ does not necessarily tend to zero with t going to infinity, the upper integration limit over t in Eq. (51) has to be chosen finite, in order to avoid divergence. We again emphasize that the above choice of ω and μ is not norm conserved in the sense that the approximate propagator P_M so

constructed does not satisfy the normalization condition (48). Of course, it is possible to minimize the error (50) with the constrain of the unit normalization, but we have to repeat this procedure at each time moment of interest. The latter requires a reasonable computational effort, if the number of time points is small enough, and becomes very arduous otherwise. Fortunately we have found that an accurate description in the entire time domain can be achieved even though the free parameters are fixed, i.e., time independent [44]. In this case, the error introduced in P_M due to the inequality $N \neq 1$ is easily reduced by a simple procedure of normalization. What is also pleasing is that the normalization of the approximate propagator P_M by itself is not far from unity and the difference $N-1$ very rapidly decreases with increasing M (see Fig. 5 in Sec. V).

Analogously, defining the error operator as $\rho^+ = \partial_t - L^+$, one gets

$$\varepsilon_A = \rho^+ A_M(\mathbf{x},t) = \xi_2 M A_M(\mathbf{x})\tau^{M+1} - (M+1)A_{M+1}(\mathbf{x})\tau^M \tag{52}$$

and

$$I_A(\omega,\mu) = \int_0^T dt \int d\mathbf{x}\ \varepsilon_A^2(\mathbf{x},t) P(\mathbf{x},0). \tag{53}$$

Minimizing the above functional provides one with a minimal (in a least-squares sense) average error of $\langle a(t)\rangle_M$ in the interval $[0,T]$ and, consequently, a reasonable choice of the free parameters for a given truncation number M. One must be cautious, however, on the use of Eq. (53) with a δ-function initial condition, in which case it provides a minimal average error in the function $A(\mathbf{x},t)$ for a given point $\mathbf{x}=\mathbf{y}$ rather than for all $\mathbf{x}$'s. The free parameters so determined usually fail to produce accurate results in the intermediate to long-time domain. A simple way of overcoming this problem is to minimize the functional (53) with the constraint

$$a_M(t\to\infty) = a_{\mathrm{st}}. \tag{54}$$

In the case that the stationary solution is not known exactly, we suggest to employ in Eq. (53), instead of $P(\mathbf{x},0)=\delta(\mathbf{x}-\mathbf{y})$, a Gaussian distribution function centered around $\mathbf{x}=\mathbf{y}$.

Fortunately, the same problem does not arise when using the global approximation (46), whose error reads

$$\begin{aligned}\varepsilon_A^g &= \rho^+ A_M^g(\mathbf{x},t) \\ &= \xi_2 M A_M(\mathbf{x})(\tau-\tau_\infty)\tau^M + \frac{M}{\tau_\infty}\left(\frac{\tau}{\tau_\infty}\right)^{M-1} \\ &\quad \times (1+\xi_1\tau+\xi_2\tau^2)[A_{st} - A_M(\mathbf{x},t\to\infty)].\end{aligned} \tag{55}$$

It is seen to go to zero as t tends to ∞ regardless of the choice of μ and ω. Therefore, the upper integration limit in Eq. (53) can be chosen infinite in this case. It is of interest that the optimal values of the free parameters thus obtained produce, more or less, accurate results with both truncation schemes discussed above. Finally, we note that a time-dependent criterion for minimizing the truncation error at each time moment t can also be constructed in an analogous fashion but we will not do so here.

V. NUMERICAL RESULTS

It will now be our aim to illustrate the power of the present formalism on a model system that is physically meaningful and simple enough to enable a comparison with exact results obtained by other means. We will deal with one of the most extensively studied problems, namely, the so-called problem of the decay of an unstable state [28,32,47–58] (see also a collection of references in Ref. [56]). It concerns a relaxation process from an initially unstable state to a final stable one that occurs in a bistable system driven by external noise. Two different cases will be distinguished. First we consider the case of Gaussian white noise with the aim to illustrate the relative efficacy of both the two-techniques presented in Secs. II and III and the two truncation schemes discussed in Sec. IV. As a second example, we consider the relaxation of an unstable system driven by exponentially correlated Gaussian noise. It is described by a two dimensional Fokker-Planck equation with a singular diffusion matrix and therefore the method outlined in Sec. III can only be tested in this case.

A. White-noise problem

A typical model repeatedly studied by many authors within this context is that governed by the one-dimensional Fokker-Planck equation

$$\partial_t P(x,t) = \partial_x(x^3 - x + D\partial_x)P(x,t), \tag{56a}$$

$$P(x,0) = \delta(x). \tag{56b}$$

It describes the dynamics of a Brownian particle that moves in the symmetric bistable potential $U(x)=x^4/4-x^2/2$, starting at the top of the barrier, in the large damping limit. The corresponding Langevin equation reads

$$\dot{x} = x - x^3 + f(t), \tag{57}$$

with $f(t)$ being Gaussian white noise normalized to

$$\langle f(t)\rangle = 0, \quad \langle f(t)f(s)\rangle = 2D\delta(t-s). \tag{58}$$

Accurate results for this model are easily obtainable for short times, e.g., by using operator decoupling techniques [32]. Exact results are also available in the long-time limit when the system reaches equilibrium

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

Beyond the above limits, there have been a number of more or less equivalent heuristic methods to handle Eq. (56) for vanishingly small fluctuations, i.e., for D tending to zero [28,32,47–56]. All these attempts, which are collectively referred to as scaling theory, have been restricted to one-dimensional systems. Moreover, their utility, with a few exceptions, is restricted to this particular equation with this

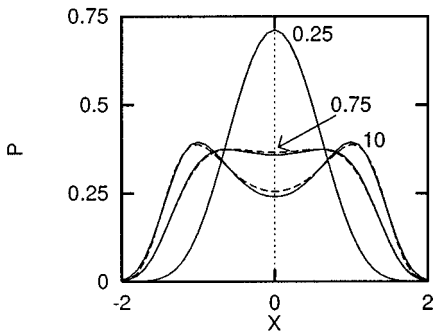

FIG. 1. Distribution function $P(x,t)$ for the model (56) for $D=0.5$ at $t=0.25$, 0.75, and 10. The solid and dashed lines are for the exact and $P_3(x,t)$ evolutions, respectively.

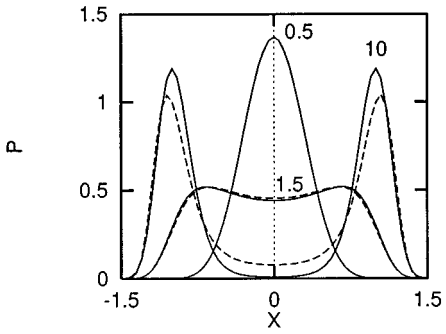

FIG. 2. Same as in Fig. 1, but for $D=0.05$ and for $t=0.5$, 1.5, and 10.

particular initial condition, and some of these solutions completely neglect fluctuations in the final regime as t goes to infinity.

These observations are in drastic contrast to the present power series expansion formalism. Apart from its generality, which has already been illustrated in quantum-mechanical, quantum-statistical, and stochastic calculations [43–45], it is both theoretically and numerically advantageous with respect to other approximate methods available in the literature in that it is rigorous and capable of extension to higher orders of approximation. The treatment is fairly straightforward and systematic and allows one to properly incorporate the true stationary solution of the considered problem. What is also important is that our formalism is not asymptotic in the noise intensity D. In particular, for $D\geqslant 0.5$ an accurate description in the *entire* time domain is already attained in the lowest-order approximations. By these we mean truncated series representations with a minimal number of terms necessary to involve all the free parameters ξ_i of the time transformation used. With the function $\tau(t)$ defined by Eq. (49) they are $P_2(x,t|y)$ and $A_3(x,t)$.

But before presenting our results we show a more simple method to evaluate the expansion coefficients of the series (33). The method is applicable when the dynamical variable can be expanded as a polynomial in x; so are the Fokker-Planck coefficients. To be specific, let us consider the Fokker-Planck equation (56a) and let the function $a(x)$ be a polynomial,

$$a(x)=\sum_{k=0}^{N}\alpha_k x^k. \tag{60}$$

Then, it is not hard to prove that the expansion coefficients $A_m(x)$ are polynomials as well,

$$A_m(x)=\sum_{k=0}^{N+2m}A_{k,m}x^k, \tag{61}$$

and their calculation is substantially simplified if one uses, in place of Eq. (34), the algebraic relation

$$mA_{k,m}=[k-\xi_1(m-1)]A_{k,m-1}-(k-2)A_{k-2,m-1}+\frac{D}{2}(k+1)(k+2)A_{k+2,m-1}-\xi_2(m-2)A_{k,m-2}. \tag{62}$$

With Eq. (62) the expansion coefficients $A_{k,m}$ are readily determined recursively starting with $A_{k,0}=\alpha_k$. The above recursive procedure is slightly different from that developed in our earlier paper [45], namely, having the expansion coefficients $A_{k,m}$ determined allows one to evaluate via Eq. (32) the time evolution of the average of a given function $a(x)$ [e.g., a given moment $\langle x^j(t)\rangle$] for any initial condition $P(x,0)$. By contrast, the recursive procedure of Ref. [45] formally provides one with all moments of the Fokker-Planck equation at once, but for a given initial condition. The generalization of Eq. (62) to arbitrary Fokker-Planck processes with polynomial coefficients is straightforward. Analogous recursion relations are also derivable for the propagator expansion, Eq. (9), but we do not present them here for the text economy.

The time evolution of the approximate distribution $P_3(x,t)$ is shown in Fig. 1 for $D=0.5$ and compared with that obtained by a finite-difference method [20]. Good agreement between approximate and numerically exact results is achieved for all times including $t\rightarrow\infty$. With decreasing D the agreement only slowly becomes worse. This is seen from Fig. 2, where an analogous comparison is given for $D=0.05$. The relative efficacy of both methods developed here is illustrated in Fig. 3 for $D=0.05$. This figure shows the relative error in the second moment made by using $P_M(x,t)$ for different truncation numbers M. Also shown are results obtained with the power series expansion for this moment $\langle x^2(t)\rangle_M$. As evidenced by Fig. 3, both approaches work equally well and provide a reasonable accuracy even in the lowest-order approximations. The corresponding (i.e., of the same order in τ) global approximations $P_M^g(x,t)$, determined by Eqs. (44) and (45), are not shown in the above figures, as these approximations are found to be almost indistinguishable from the numerically exact results; so are the global approximations for the second moment determined through Eq. (46). In order to demonstrate the relative efficacy of the ordinary truncation scheme and that based on the true stationary solution, we present in Fig. 4 the relative error in the second moment made by using $\langle x^2(t)\rangle_M$ and

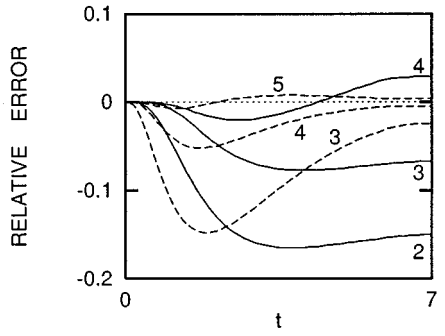

FIG. 3. Relative error, [(approximate)−(exact)]/(exact), in the second moment $\langle x^2(t)\rangle$ for the model (56) for $D=0.05$. Dashed lines, results obtained with the power series expansion for the moment $\langle x^2(t)\rangle_M$ for $M=3$, 4, and 5; solid lines, results of the series expansion for the propagator $P_M(x,t)$ for $M=2$, 3, and 4.

$\langle x^2(t)\rangle_M^g$ for different truncation numbers M and for $D=0.05$ and 0.01. For the sake of comparison these calculations have been carried out with one and the same time transformation given by $\mu=\omega=1$. It is seen that successive higher orders reduce the error over a larger range of t and yet the results obtained with the global approximation $\langle x^2(t)\rangle_M^g$ [Eq. (46)] are much more accurate than those of the corresponding ordinary truncation scheme $\langle x^2(t)\rangle_M$. It is also worthwhile noticing the sensitivity of the convergence rate to the choice of the free parameters. As evidenced by Fig. 3,

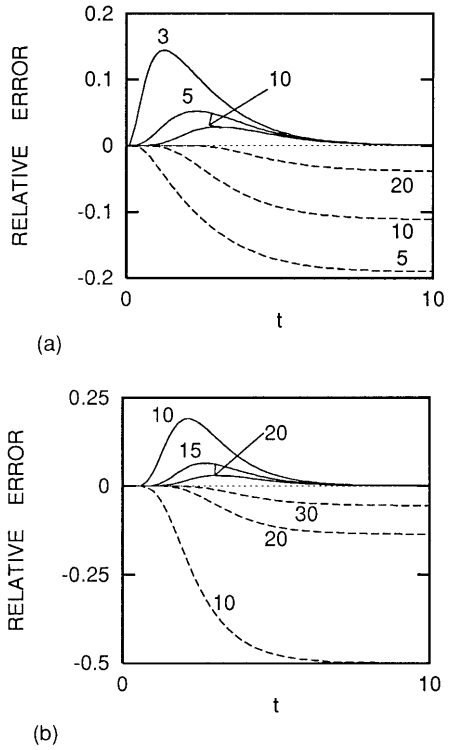

FIG. 4. Relative error in the second moment $\langle x^2(t)\rangle$. The dashed and solid lines show, respectively, the error of the ordinary truncation scheme $\langle x^2(t)\rangle_M$ and that of the global approximation $\langle x^2(t)\rangle_M^g$ obtained with different truncation numbers M. (a) $D=0.05$ and (b) $D=0.01$.

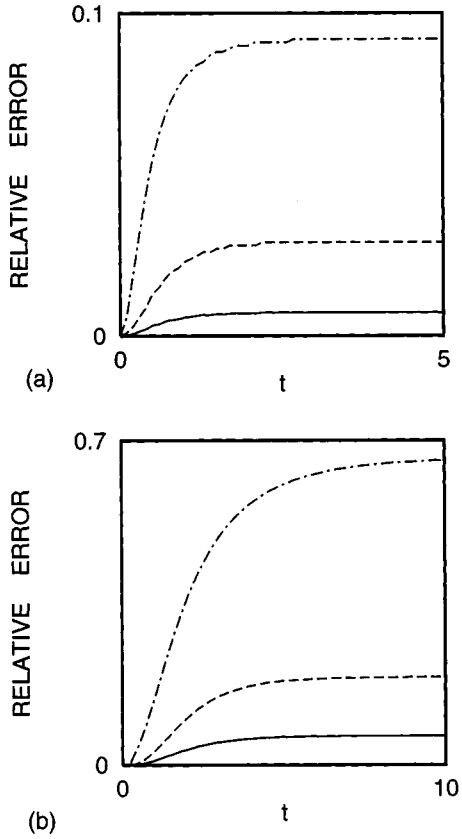

FIG. 5. Relative error in the normalization [Eq. (63)] for the model (56). The dashed, dot-dashed, and solid lines are, respectively, for the results obtained using $P_M(x,t)$ with $M=2$, 3, and 4. (a) $D=0.5$ and (b) $D=0.05$.

should the free parameters be determined by Eqs. (53) and (54), the power series representation $\langle x^2(t)\rangle_M$ converges sufficiently rapidly and a very accurate description is already attained for $M=5$. By contrast, with the time transformation given by $\mu=\omega=1$, an analogous level of accuracy in $\langle x^2(t)\rangle_M$ is achieved only for $M>20$ [see Fig. 4(a)].

Finally, we recall that the present choice of free parameters is not norm conserved. The same is true for the various different numerical schemes available in the literature for solving Fokker-Planck and Schrödinger equations, most of which do not preserve the norm of the solution (see, e.g., [3,9,10,14,17]). It is well known, however, that a dramatic reduction of normalization error is already attained just by replacing $P_M(x,t)$ by $P_M(x,t)/N(t)$, where $N(t)$ reads

$$N(t)=\int_{-\infty}^{\infty} dx\ P_M(x,t). \tag{63}$$

The accuracy achieved with this simple procedure seems encouraging (see Figs. 1, 2, and 3). Thus the interesting issue it remains to discuss is the following: How large is the error in N as a function of the truncation order M? This issue is addressed in Fig. 5, which shows the relative error in the normalization of the approximate propagator $P_M(x,t)$, obtained for different truncation numbers M, as a function of time. The calculations are performed for $D=0.5$ and 0.05 with $\mu=\omega=2$ and $\mu=\omega=0.45$, respectively. This error is

seen to increase with D going to zero, but each successive higher order reduces it considerably.

B. Colored-noise problem

As a second and more challenging example, we consider the relaxation of an unstable system driven by a noise with a finite correlation time. To be specific we restrict the discussion to a system governed by the Langevin equation

$$\dot{x}=x-x^3+v(t), \tag{64}$$

where the driving noise term $v(t)$ is modeled as the stationary Ornstein-Uhlenbeck process

$$\dot{v}=\gamma[-v+f(t)], \tag{65}$$

with γ^{-1} being the correlation time of the noise. The white-noise term $f(t)$ appearing in the above equation is defined by Eq. (58). As $f(t)$ is Gaussian and has a zero mean, the noise $v(t)$ is also Gaussian with statistical properties

$$\langle v(t)\rangle=0, \quad \langle v(t)v(s)\rangle=D\gamma\exp(-\gamma|t-s|). \tag{66}$$

When γ goes to infinity (short correlation times), one can completely neglect the term $\dot{v}$ in Eq. (65), thus reducing the problem to that already studied in Sec. V A. For finite γ's the Fokker-Planck equation describing the pair stochastic process (x,v) reads

$$\partial_t P(x,v,t)=[\partial_x(x^3-x-v)+\gamma\partial_v(v+D\gamma\partial_v)]P(x,v,t). \tag{67}$$

Since the noise is assumed to be stationary, its probability distribution is given by

$$P_v(v)=(2\pi\gamma D)^{-1/2}\exp\left(\frac{-v^2}{2\gamma D}\right). \tag{68}$$

Assuming further that x and v are statistically independent at $t=0$, one can write their joint distribution as

$$P(x,v,0)=\delta(x)P_v(v). \tag{69}$$

We note that the above problem has already been studied in Refs. [57,58], and two approximate solutions have been obtained. Both solutions are asymptotically valid in the limit of vanishingly small D, being a straightforward extension of the scaling theory to systems driven by an Ornstein-Uhlenbeck noise. We also note that the diffusion matrix of Eq. (67) does not possess an inverse, while the equation itself does not obey detailed balance. The former means that the power series representation of the propagator, Eq. (9), is not applicable in this case, while the latter property prevents us from making use of the truncation scheme based on the true stationary solution, as this solution is not known exactly.

Our aim is to illustrate the utility of the method outlined in Sec. III in treating situations of such a kind. The moments of Eq. (67), $\langle x^k(t)v^r(t)\rangle$, can be calculated in terms of Eqs. (33) and (34). Since, however, the function $a(x,v)=x^k v^r$ and the Fokker-Planck coefficients are polynomials in the considered case, the expansion coefficients $A_m(x,v)$ are also polynomials,

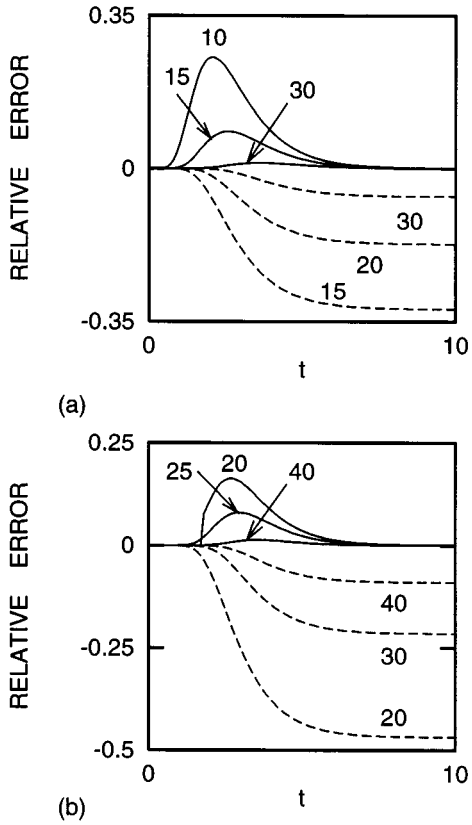

FIG. 6. Same as in Fig. 4, but for a colored-noise problem [Eqs. (67) and (69)] for $D=0.01$. (a) $\gamma=5$ and (b) $\gamma=0.5$.

$$A_m(x,v)=\sum_{i=0}^{k+2m}\sum_{j=0}^{r+m}A_{i,j,m}x^i v^j, \tag{70}$$

and their calculation is substantially simplified if one uses, instead of Eq. (34), the algebraic relation

$$\begin{aligned} mA_{i,j,m}=&[i-\gamma j-\xi_1(m-1)]A_{i,j,m-1}+(i+1)A_{i+1,j-1,m-1}\\ &-(i-2)A_{i-2,j,m-1}+D\gamma^2(j+1)(j+2)A_{i,j+2,m-1}\\ &-\xi_2(m-2)A_{i,j,m-2}. \end{aligned} \tag{71}$$

In particular, with Eq. (69) the moments of the stochastic process are obtained by a series

$$\langle x^{2k+1}(t)\rangle=0,$$

$$\langle x^{2k}(t)\rangle=\sum_{m=0}\sum_{j=0}^{m/2}(2j-1)!!A_{0,2j,m}(\gamma D)^j\tau^m. \tag{72}$$

Numerically exact results for these moments were obtained by a path-integral method described earlier [32] for the choice of parameters $D=0.01$ and $\gamma=5$ and 0.5. Figure 6 shows the relative error made by using $\langle x^2(t)\rangle_M$ for different truncation numbers M. Also shown is the error obtained with the global approximation $\langle x^2(t)\rangle_M^g$. The latter is constructed in terms of the numerically exact results. For the sake of comparison, the calculation is again performed with $\mu=\omega=1$. As expected, for $\gamma=5$ the rate of convergence of the present method is almost the same as in the white-noise

limit $\gamma=\infty$ [cf. Figs. 4(b) and 6(a)]. In both cases, an adequate level of accuracy in the entire time domain is achieved for $M\sim 30$. With decreasing γ the convergence slowly becomes worse [cf. Figs. 6(a) and 6(b)]. The reason is that the expansion coefficients also become smaller in this case, and a larger number of terms has to be included in the series (72) to obtain convergent results in the long-time limit.

One can thus conclude that the present power series expansion formalism offers a powerful tool for systematically treating nonequilibrium statistical mechanics. It is a method that can be applied to simple or complex systems and high dimensionality does not seem to present special problems. We also note the relative ease with which this method can be implemented. Almost all calculations are doable analytically in a simple, economical way, thus allowing one to get accurate results with minimal computational efforts. From this point of view the present method is both theoretically and numerically advantageous with respect to the various approximate algorithms available for numerically integrating the Fokker-Planck equation (1).

VI. CONCLUSION

In this work, the power series expansion formalism is developed for general Fokker-Planck-Schrödinger processes. The idea introduced here is directly applied to deriving power series representations for the propagator and for the average of dynamical variables. Recursion relations are obtained for the expansion coefficients that can be *analytically* evaluated for any number of degrees of freedom. The recursive evaluation of the expansion coefficients can be carried out systematically until a given level of accuracy is reached. The treatment is fairly straightforward and allows one to properly incorporate the true long-time limit solution of the problem under study whenever that is known exactly. In the event that there is no closed-form solution of the stationary problem, an approximate stationary (ground-state) solution can be obtained recursively from the expansion for the propagator, Eq. (9), taken at $\mathbf{y}=\mathbf{x}$ in the limit $t=\infty$. The corresponding free parameters are determined variationally, e.g., by minimizing the error functional

$$I_P(\omega,\mu)=\int d\mathbf{x}[LP(\mathbf{x},\infty|\mathbf{x})]^2. \tag{73}$$

This is of interest considering the lack of a satisfactory analytical description for the stationary properties of a diffusion process without detailed balance [2]. Analogous results are also derivable by application of the power series expansion method outlined in Sec. III. Two general approaches are possible in such a case: One can use a cumulant generating function formalism [14] or develop a variational scheme for reconstructing a distribution function in terms of known averages [59]. These approaches are planned to be discussed at greater length in a future paper.

Another problem of importance refers to the classical rate theory. The thermally activated escape over a barrier represents a decisive step in the dynamics of various processes in physics, chemistry, and biology, and a great deal of effort has been devoted in recent times in order to determine the transition rate over the barrier [60]. General expressions for this rate are derived by linearizing the original Fokker-Planck operator in the vicinity of the barrier top [61]; however, they are valid if and only if the potential barrier ΔU is sufficiently large when compared to the energy of thermal motion β^{-1}, so that there are no other quantities that are comparable or smaller than $(\beta\Delta U)^{-1}$. If this is not the case, the rate expressions may fail grossly [7]. One also notes that a perturbation procedure that has recently been developed for obtaining finite barrier corrections of the rate [62] is too complicated to be useful beyond second order in $(\beta\Delta U)^{-1}$. By contrast, the power series formalism developed here offers a convenient tool for systematically treating the escape problem both analytically and numerically. Aside from the two aforementioned examples that are currently investigated by the present author, this formalism can be applied to many other fields involving Fokker-Planck, Bloch, and Schrödinger equations.

ACKNOWLEDGMENT

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