Distributed approximating functional approach to the Fokker–Planck equation: Time propagation

G. W. Wei,[a)] D. S. Zhang,[b)] and D. J. Kouri[c)]
Department of Chemistry and Department of Physics, University of Houston, Houston, Texas 77204-5641

D. K. Hoffman
Department of Chemistry and Ames Laboratory,[d)] Iowa State University, Ames, Iowa 50011

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The Fokker–Planck equation is solved by the method of distributed approximating functionals via forward time propagation. Numerical schemes involving higher-order terms in Δt are discussed for the time discretization. Three typical examples (a Wiener process, an Ornstein–Uhlenbeck process, and a bistable diffusion model) are used to test the accuracy and reliability of the present approach, which provides solutions that are accurate up to ten significant figures while using a small number of grid points and a reasonably large time increment. Two sets of solutions for the bistable system, one computed using the eigenfunction expansion of a preceding paper and the other using the present time-dependent treatment, agree to no fewer than five significant figures. It is found that the distributed approximating functional method, while simple in its implementation, yields the most accurate numerical solutions yet available for the Fokker–Planck equation. © *1997 American Institute of Physics.* [S0021-9606(97)52731-0]

I. INTRODUCTION

One of the difficult outstanding theoretical problems in statistical mechanics is the relation between macroscopic irreversibility and microscopic reversibility. The Fokker–Planck equation (FPE), as a mesoscopic kinetic equation incorporating a deterministic drift vector and a chaotic diffusion tensor, provides a conceptual framework for the understanding of our macroscopic world in terms of microscopic principles. More and more phenomena have been found that are described by the Fokker–Planck equation. The simplicity and range of application of the Fokker–Planck equation makes it a highly popular kinetic equation, both for theoreticians and for experimentalists. On one hand, theoretical aspects of the Fokker–Planck equation, in some cases stimulated by new experimental findings, are still under intensive study. On the other hand, a variety of new experimental phenomena, motivated by theoretical predictions, are found to be well described by the Fokker–Planck equation. In addition to work prompted by this synergy between theory and experiment, there is another line of inquiry that involves intensive efforts to solve the Fokker–Planck equation accurately and efficiently. Analytical solutions are limited to only a few simple cases, which are valuable in their own right, and for testing new numerical methods. For more complicated problems, both analytical analyses and numerical methods are indispensable since the former yield a conceptual basis for understanding and the latter provide detailed solutions.

Various approaches have been explored for numerical solution of the Fokker–Planck equation. Path integral methods have been utilized by a number of authors.[1–3] Wehner and Wolfer[4] have presented an elegant formalism where one numerically evaluates the path integrals involving the Onsager–Machlup functionals.[5] Monte Carlo techniques[6] are useful for providing information about certain properties of the system, in terms of the moments of the underlying stochastic process, without the need for direct reference to the probability density distribution. In the case where the entire distribution function is required, direct approaches, such as the finite difference method, are frequently used.[7–9] However the finite difference method often leads to stiff (with respect to time) systems of ordinary differential equations. Chang and Cooper[10] were the first to discuss a practical finite difference procedure that allows the distribution function to evolve in a quasiequilibrium manner, preserving the number density of the system in the absence of external sources or sinks. Larsen *et al.*[11] have recently generalized the Chang–Cooper method to increase the time increment and to achieve greater numerical stability for a wide class of systems, including the nonlinear Compton scattering problem. Their approach, however, depends on having analytic expressions for the collision parameters, which may not be available for practical application. More recently, Epperlein[12] further generalized the Chang–Cooper method by taking into account energy conservation. His fully conservative scheme has been successfully applied to the Coulomb collision problem for a spatially homogeneous plasma. It is noted that the kinetic theory for an open system obviously does not require number density or energy conservation, which is the case where sinks and sources are present. Scaling theory[13] and normal mode analysis[14] are also useful for obtaining approximate solutions. For a general class of problems, the eigenvalue expansion method is applicable.[15,16] In this approach, various spectral methods can provide extremely accurate results for the

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Fokker–Planck equation. In particular, Shizgal's method,[15] using nonclassical weight functions, especially adapted to the problem under study, has been shown[16] to be superior to most other methods in terms of accuracy.

In a previous paper[17] we applied the distributed approximating functional (DAF) method[18,19] to the solution of the linearized Fokker–Planck equation using eigenfunction expansion. Three examples (a Lorentz Fokker–Planck equation, a bistable diffusion model, and a Henon–Heiles two-dimensional anharmonic resonating system) were used for numerical testing. All results obtained were in excellent agreement with those of established methods, and, in particular, with the results of Shizgal's method.[15,16] It was found that the distributed approximating functional method yields accuracy of the same order as a spectral method but possesses a local method's simplicity and flexibility for the eigenvalue problems arising from the Fokker–Planck equations. In general, the eigenfunction expansion solutions calculated through the DAF method are very accurate. The full time-dependent solutions of the Fokker–Planck equation are, of course, obtained as long as the complete set of eigenfunctions and expansion coefficients are calculated for a given initial distribution. However, in the case where the eigenfunction expansion method cannot be applied, such as when the effective potentials of the Schrödinger-like Fokker–Planck equation do not support any bound states, a different method is required. In the present paper we discuss an alternative DAF approach for solving the time-dependent, linearized Fokker–Planck equation, namely a time-dependent wave packet propagation scheme. Three different examples are considered in the present study. Rigorous error analyses indicate that the present time-dependent DAF approach, while being extremely simple and easy to implement, provides some of the most accurate solutions yet available to the Fokker–Planck equation. Extremely high accuracy is required if one is to simulate extremely high resolution spectroscopic measurements [for example, a modern Fourier transform infrared spectrometer can easily provide a resolution down to 0.004 cm^{-1} for wave numbers on the order of several thousands of cm^{-1} (or one part in 10^6), even for unstable van der Waals molecules]. Similarly, spectroscopic measurements of alkali dimers in Bose–Einstein condensation experiments are accurate to at least six significant figures. Another instance requiring extremely high accuracy occurs when one is solving a general class of nonlinear partial differential equations, such as the nonlinear Fokker–Planck equation, where bifurcations can occur. Yet another arises when one is treating a system involving irregular boundaries, such as the problem of diffusion in the midst of macromolecules. Therefore, it is important to develop numerical methods that are capable of handling such challenges. In other test calculations, our results indicate that an alternative DAF approach provides the most accurate results for a nonlinear Fokker–Planck equation[20] and for the nonlinear Burgers' equation in one- and two-space dimensions.[21] It also provides the first ever results for the two-dimensional Kuramoto–Sivashinsky equation with an irregular finite boundary.

This paper is organized as follows: The theoretical basis for the present work is briefly reviewed in Sec. II. We refer the reader to our earlier paper for additional details on the Fokker–Planck equation and the DAF formalism. The emphasis of our presentation is on a number of numerical schemes involving higher-order terms in Δt, which may be contrasted with the stochastic derivation of the Fokker–Planck equation.[5] The DAF form of a more general operator, namely the Kramers–Moyal operator,[22,23] of which the Fokker–Planck operator is a special case, is also presented and discussed. The numerical analyses and results of the present DAF approach, as illustrated through three examples, are the subjects of Sec. III. We first consider a Wiener process that is one of few cases for which analytical solutions of the Fokker–Planck equation are available. This is particularly important for developing new solution methods since every new numerical method needs to be tested by application to some problems for which the exact solution is known. To test further the accuracy and the reliability of the present DAF approach, we consider a second exactly soluble system that has also been used as a standard test problem for evaluating various new numerical methods, namely the Ornstein–Uhlenbeck process.[24] Unlike the Wiener process, this example has not only a random fluctuation term, but also a nonvanishing linear drift term, and thus it captures the essence of general Fokker–Planck equations. The last test problem studied in this work is the same bistable system that was used in our earlier paper. This problem has been especially selected for the following reasons. First, the bistable system is physically important in the theory of the Fokker–Planck equation and has received an enormous amount of attention in the literature.[25,13,26,27] Second, it has been used as an example for illustrating different numerical methods. Finally, it is interesting that the DAF formalism is capable of providing two completely different approaches, namely, the eigenfunction expansion and the time-dependent propagation treatment, to the same Fokker–Planck equation. We report a self-consistency check to verify that the two DAF solutions obtained using different methods agree. A brief conclusion is given at the end of this paper.

II. THEORETICAL BACKGROUND

It is well known that the Fokker–Planck equation can be obtained by a reduction of more rigorous kinetic equations, such as the BBGKY hierarchy, the Boltzmann equation, or from stochastic theory.[25,5] We consider a process in which $P(x,t)$ and $P(x,t+\Delta t)$, the probability densities at time t and a later time $t+\Delta t$, respectively, are related to each other by a transition probability $P(x,t+\Delta t|y,t)$,

$$P(x,t+\Delta t)=\int P(x,t+\Delta t|y,t)P(y,t)dy. \tag{1}$$

If the process is Markovian, the transition probability can be rewritten using a Taylor expansion, as

$$P(x,t+\Delta t|y,t)=\left\{1+\sum_{n=1}\left[\left(-\frac{\partial}{\partial x}\right)^n\frac{M_n(x,t,\Delta t)}{n!}\right]\right\}\times\delta(x-y),\tag{2}$$

where the moment $M_n(x,t,\Delta t)$ of the transition probability is standardly defined as

$$M_n(x,t,\Delta t)=\int (y-x)^n P(y,t+\Delta t|x,t)dy.\tag{3}$$

This function is assumed to be expandable with respect to a small time increment, Δt, according to

$$M_n(x,t,\Delta t)=n!A_n(x,t)\Delta t+O[(\Delta t)^2].\tag{4}$$

To the first-order approximation in Δt, the equation of the change of the probability density $P(x,t)$ is

$$\frac{\partial P(x,t)}{\partial t}=\sum_{n=1}\left(-\frac{\partial}{\partial x}\right)^n A_n(x,t)P(x,t)=L_{\mathrm{KM}}P(x,t),\tag{5}$$

where Eqs. (2)–(4) have been used. Equation (5) is known as the Kramers–Moyal forward expansion and, correspondingly, L_{KM} is the Kramers–Moyal operator,[22,23] which is, in general, *time dependent*. The Fokker–Planck equation follows if the Kramers–Moyal expansion is truncated at second order,[28]

$$\frac{\partial f(x,t)}{\partial t}=\frac{\partial[A(x,t)f(x,t)]}{\partial x}+\frac{\partial^2[B(x,t)f(x,t)]}{\partial x^2}\equiv L_{\mathrm{FP}}f(x,t),\tag{6}$$

where we have replaced the probability density $P(x,t)$ with the distribution function $f(x,t)$. L_{FP} is the Fokker–Planck operator, which also is time dependent. In the case where L_{KM} is independent of time, the formal solution of Eq. (5) is given by

$$P(x,t)=\exp(L_{\mathrm{KM}}t)P(x,0).\tag{7}$$

In the general time-dependent situation, Eq. (7) can be used as a convenient starting point for path integral methods. In any case, for a small time increment Δt, the approximate solution of Eq. (5) is often written as[5]

$$P(x,t+\Delta t)=\{1+L_{\mathrm{KM}}\,\Delta t+O[(\Delta t)^2]\}P(x,t),\tag{8}$$

in agreement with the approximation (4) used in the derivation of Eq. (5). Similarly, for the solution of the Fokker–Planck equation (6), one has

$$f(x,t+\Delta t)=\{1+L_{\mathrm{FP}}\,\Delta t+O[(\Delta t)^2]\}f(x,t).\tag{9}$$

It is particularly important to note that, while both Eqs. (8) and (9) are conceptually correct, neither of them provides a practical starting point for numerical applications. Keeping only linear terms in Δt will provide a good approximation to Eq. (5) or the Fokker–Planck equation *only* in the limit $\Delta t\rightarrow 0$. This is obviously often impractical from the numerical point of view. Instead, for computations using Eqs. (8) and (9), we can write the Rth-order approximation as

$$P(x,t+\Delta t)\approx\left(1+\sum_{n=1}^{R}\frac{1}{n!}L_{\mathrm{KM}}^n(\Delta t)^n\right)P(x,t),\tag{10}$$

and for the solution of the Fokker–Planck equation (9),

$$f(x,t+\Delta t)\approx\left(1+\sum_{n=1}^{R}\frac{1}{n!}L_{\mathrm{FP}}^n(\Delta t)^n\right)f(x,t).\tag{11}$$

Various-order approximations to the solutions of the Fokker–Planck equations are examined in this work.

For the present computations, one can easily construct the Hermite DAF representation of the Kramers–Moyal operator L_{KM} as

$$L_{\mathrm{KM}}(x_i,x_j;t)=\sum_{n=1}(-1)^n\sum_{l=0}^{n}\frac{n!}{(n-l)!l!}A_n^{(n-l)}(x_i,t)\frac{\Delta}{2^{1/2}\sigma^{l+1}}\exp\left(\frac{-(x_i-x_j)^2}{2\sigma^2}\right)\times\sum_{m=0}^{M/2}\left(\frac{-1}{4}\right)^m(-1)^l\frac{1}{\sqrt{2\pi}m!}\times H_{2m+l}\left(\frac{x_i-x_j}{\sqrt{2}\sigma}\right),\tag{12}$$

where Δ is the spatial grid spacing. Obviously, the Hermite DAF representation of the Fokker–Planck operator L_{FP} follows as a special case of Eq. (12).

In the case where the generalized diffusion coefficient is a constant with respect to position, as is true for the Ornstein–Uhlenbeck process, the time evolution of the diffusion operator takes on a particularly simple form in the Hermite DAF representation, namely

$$\exp\left(\alpha\frac{d^2}{dx^2}t\right)f_{\mathrm{M}}(x)=\int_{-\infty}^{\infty}dx'\,F_{\mathrm{DAF}}(x-x'|t)f(x'),\tag{13}$$

where $F_{\mathrm{DAF}}(x-x'|t)$ is given by[18]

$$F_{\mathrm{DAF}}(x-x'|t)=\frac{1}{\sigma}\exp\left(\frac{-(x-x')^2}{2\sigma_t^2}\right)\times\sum_{n=0}^{M/2}\left(\frac{-1}{4}\right)^n\left(\frac{\sigma}{\sigma_t}\right)^{2n+1}\frac{1}{\sqrt{2}\pi n!}\times H_{2n}\left(\frac{x-x'}{\sqrt{2}\sigma_t}\right),\tag{14}$$

and σ_t, as a function of evolution time t, is

$$\sigma_t^2=\sigma^2+2\alpha t.\tag{15}$$

The operator, $\exp(L_{\mathrm{FP}}\,\Delta t)$ [cf. Eq. (7)], can be written in the symmetric split operator form [accurate to $O(\Delta t^2)$] to obtain

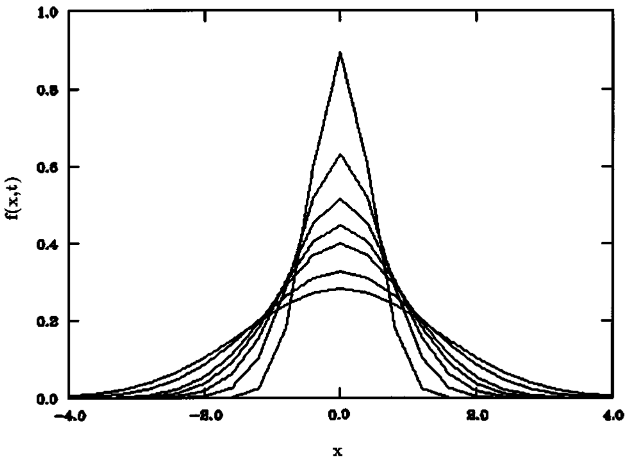

FIG. 1. The exact and numerical solutions ($N=50$, $\Delta t=0.01$, $R=2$) of the Wiener process. The centerlines in the descending order are at $t=0.2;0.4;0.6;0.8;1.0;1.5;2.0$. The initial delta distribution is at $x=0.0$.

TABLE I. Errors of solutions for the Wiener process.

Time	$R=2$		$R=4$	
	L_2	L_∞	L_2	L_∞
0.2	7.34(−04)	8.18(−04)	3.66(−04)	1.85(−04)
0.3	2.48(−04)	3.14(−04)	7.41(−05)	3.58(−05)
0.4	1.18(−04)	1.36(−04)	8.07(−06)	4.09(−06)
0.5	7.06(−05)	7.49(−05)	7.98(−07)	4.46(−07)
0.6	4.64(−05)	4.68(−05)	9.06(−08)	6.09(−08)
0.7	3.26(−05)	3.16(−05)	1.47(−08)	1.10(−08)
0.8	2.40(−05)	2.25(−05)	3.96(−09)	2.71(−09)
1.0	1.45(−05)	1.28(−05)	1.16(−09)	9.35(−10)
1.5	5.76(−06)	4.61(−06)	2.03(−10)	1.63(−10)
2.0	3.00(−06)	2.23(−06)	5.95(−11)	4.44(−11)

$$f(x,t+\Delta t)\approx\left[1+\sum_{n=1}^{R}\frac{1}{2n!}\left(\frac{\partial A(x,t+\Delta t)}{\partial x}\Delta t\right)^n\right]\times\exp\left(B\frac{\partial^2}{\partial x^2}\Delta t\right)\times\left[1+\sum_{n=1}^{R}\frac{1}{2n!}\left(\frac{\partial A(x,t+\Delta t)}{\partial x}\Delta t\right)^n\right]f(x,t). \tag{16}$$

The spatial integration, implied by Eq. (13), can be performed by quadrature. The exponential term in the middle is easily expressed analytically in the DAF representation [see Eq. (14)]. This scheme has also been tested for the Ornstein–Uhlenbeck process in the present work.

III. NUMERICAL APPLICATIONS

We illustrate the DAF-based time-dependent approaches to the Fokker–Planck equation through three standard examples, with natural boundary conditions. The accuracy of the present DAF treatment is assessed by comparing its results with solutions obtained by exact methods, and by comparing to the earlier DAF eigenfunction expansion approach.[17] The present time-dependent DAF approach, for the problems we have studied, is more accurate than other time-dependent approaches.[4,9,28] The details of the present study are given in the following three sections. The Hermite DAF parameters are taken as $M=88$ and $\sigma=3.05\Delta$ for all example calculations reported in this work.

A. Wiener process

The so-called Wiener process is a statistical model for a nonstationary Markov process. The Fokker–Planck equation governing it is simply a classical diffusion equation,

$$\frac{\partial f(x,t)}{\partial t}=D\frac{\partial^2 f(x,t)}{\partial x^2}, \tag{17}$$

where D is the diffusion coefficient. With an initial δ-function distribution localized at x_0, the analytical solution of Eq. (17) is

$$f(x,t)=\sqrt{\frac{1}{4D\pi(t-t_0)}}\exp\left(-\frac{(x-x_0)^2}{4D(t-t_0)}\right). \tag{18}$$

Despite the simplicity of Eq. (18), the Wiener process is conceptually important for stochastic theory.[25] It has been used as a standard example for testing numerical methods. Wehner and Wolfer[4] applied their path-integral method to this process and obtained errors of a few percent in their solutions. The time-dependent solution for this system can be obtained analytically with the DAF propagator given in Eq. (13). However, since this treatment cannot be used in more general applications, we will not pursue it further. Our interest here is to test the more general time-dependent scheme of Eq. (11) by varying the order (R) of approximation. The present solutions are obtained by using the second-order and fourth-order approximations with a time increment of $\Delta t=0.01$. The computation is conducted using a sufficiently large interval $[-10,10]$ of coordinate space to ensure that boundary reflection is negligible. Fifty grid points ($N=50$) are used for this interval and the initial δ function is localized at $x=0$. As shown in Fig. 1, the exact solutions and numerical solutions are graphically indistinguishable. Therefore, we do both L_2 and L_∞ error analyses to evaluate the quality of the various DAF-based methods, the results of which are listed in Table I. It is noted that the unsmooth feature in Fig. 1, as well as in some other figures, reflects the fact that very few grid points are used in our computations. To our knowledge, the present time-dependent DAF approach provides the most accurate numerical results yet obtained. For the time increment used, the fourth-order approximation ($R=4$) is significantly more accurate than the second approximation ($R=2$) at all times. It is true that, consistent with the derivation of the Fokker–Planck equation, this difference will diminish as the time increment is made sufficiently small. However, computationally, it is more efficient to use higher-order expansions than to decrease the time increment since the former reduces the number of applications of the propagator. Another trend seen in Table I is that the errors decrease as time increases. This is due to the poor numerical

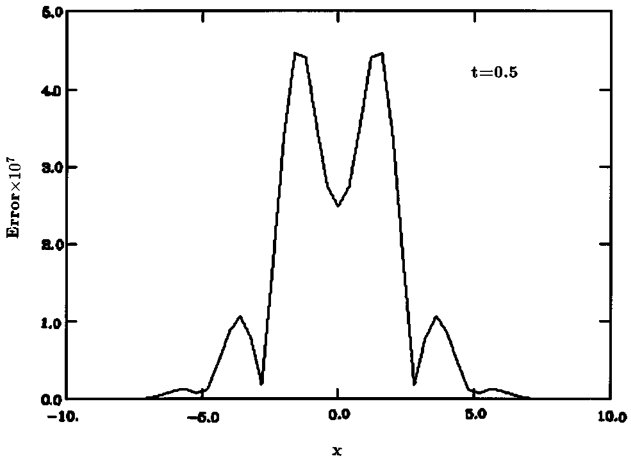

FIG. 2. The pointwise errors of the solution $f(x,0.5)$ for the Wiener process ($N=50$, $\Delta t=0.01$, $R=4$).

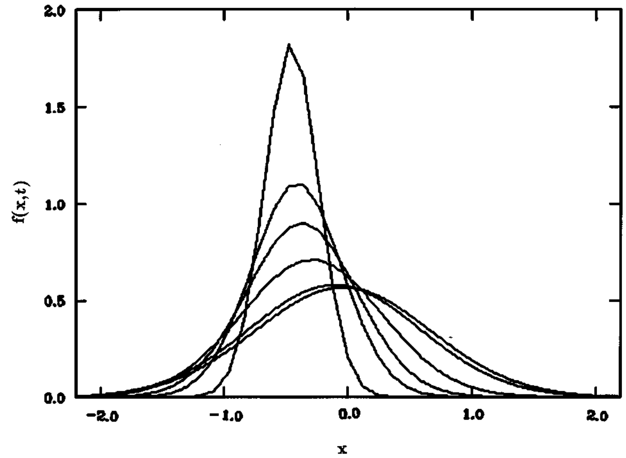

FIG. 3. The exact and numerical solutions ($N=50$, $\Delta t=0.05$, $R=4$) of the Orstein–Uhlenbeck process. The lines in the descending order are at $t=0.2;0.6;1.0;2.0;6.0;10.0$. The initial delta distribution is at $x=-0.416$.

representation of the initial Dirac delta function. Obviously had one started with a smooth initial *wave packet*, or used more grid points, one would have obtained much higher accuracy at earlier times as well. We have verified this computationally, but these results are not presented. The poor numerical representation of the delta function can be seen from the plots of pointwise error distributions. Such a plot for $t=0.5$ is given in Fig. 2. It is seen that most of the error occurs around the initial ''delta function'' position. It has also been noted that this is true for other times as well.

B. Ornstein–Uhlenbeck process

The Ornstein–Uhlenbeck process is a stationary Markov process describing a linear drift-diffusion system, and is characterized by

$$A_1(x)=\gamma x; \quad A_2(x)=D, \tag{19}$$

where γ and D are positive constants. The Fokker–Planck equation for the process is

$$\frac{\partial f(x,t)}{\partial t}=\gamma\frac{\partial[xf(x,t)]}{\partial x}+D\frac{\partial^2 f(x,t)}{\partial x^2}. \tag{20}$$

With an initial delta function distribution localized at x_0, the exact solution of the Ornstein–Uhlenbeck Fokker–Planck equation is a Gaussian,

$$f(x,t)=\left(\frac{\gamma}{2D\pi\sqrt{(1-e^{-2\gamma(t-t_0)})}}\right)\times\exp\left(-\frac{\gamma(x-x_0e^{-2\gamma(t-t_0)})^2}{2D(1-e^{-2\gamma(t-t_0)})}\right). \tag{21}$$

A stationary Gaussian distribution results in the limit when $\gamma(t-t_0)\gg 1$. The Ornstein–Uhlenbeck process has various physical applications, such as a laser field far below (or above) its threshold,[5] a linear overdamped oscillator in the presence of colored Gaussian noise,[29] and the velocity relaxation of a Rayleigh gas.[30] The equation is also computationally important and has been used for testing various new numerical schemes.[16,4] In the present computations, γ and D are chosen to be 0.25 and 0.125, respectively. In an interval of $[-5.2, 5.2]$, two sets of grid points ($N=50$, 100) are used with the initial delta functions located at -0.416 and -0.520, respectively. The time increments used for $N=50$ and $N=100$ are 0.05 and 0.01, respectively. Both exact solutions and (graphically identical) numerical solutions are plotted in Fig. 3, for a few different times. We also test the second- ($R=2$) and fourth-($R=4$) order approximations according to Eq. (11). The L_2 and L_∞ errors for a variety of solutions are listed in Table II. It is evident that the time-dependent DAF approach is able to provide extremely high accuracy while using a relatively small number of grid points and reasonably large time increments. Basic accuracy trends can be summarized as follows: more grid points yield higher accuracy and accuracy improves with increasing time. It is noted that the time-dependent DAF approach provides *enough* accuracy for most practical purposes, even if one only chooses the second-order approximation ($R=2$) and employs a small number of grid points with a very large time step ($\Delta t\approx 0.05$). As seen from Fig. 4, the largest pointwise errors occur in the neighborhood of the position of the initial localized distribution. We expect that an increase in accuracy for the earlier time solutions can be further achieved if the initial delta functions are replaced by numerically smoother functions. We have also examined the split operator scheme (16) for this system and preliminary results indicate that it is not as accurate as the other schemes used in this section. A more detailed study is needed, however, to justify a final conclusion regarding the split operator approach. We leave this for future work.

C. A bistable system

To demonstrate further the reliability and robustness of the time-dependent DAF method for the Fokker–Planck

TABLE II. Errors of solutions for the Ornstein–Uhlenbeck process.

Time	Second-order approximation $N=50$, $\Delta t=0.05$ L_2	L_∞	Second-order $N=100$, $\Delta t=0.01$ L_2	L_∞	Fourth-order approximation $N=50$, $\Delta t=0.05$ L_2	L_∞	Fourth-order $N=100$, $\Delta t=0.01$ L_2	L_∞
0.1	1.22(−01)	1.62(−01)	5.08(−03)	1.26(−02)	1.49(−02)	2.02(−02)	6.92(−05)	1.45(−04)
0.2	5.80(−02)	8.62(−02)	8.46(−04)	1.63(−03)	3.62(−03)	3.62(−03)	1.81(−06)	3.47(−6)
0.3	1.95(−02)	3.29(−02)	3.21(−04)	5.56(−04)	7.18(−04)	8.68(−04)	2.97(−07)	5.15(−07)
0.6	1.98(−03)	3.29(−03)	6.30(−05)	9.26(−05)	2.18(−05)	2.63(−05)	1.42(−08)	2.10(−08)
1.0	5.28(−04)	7.20(−04)	1.91(−05)	2.52(−05)	1.46(−05)	1.75(−05)	1.54(−09)	2.04(−09)
2.0	9.63(−05)	1.14(−04)	3.72(−06)	4.30(−06)	1.21(−05)	1.24(−05)	7.73(−11)	8.70(−11)
4.0	2.13(−05)	1.77(−05)	6.90(−07)	7.17(−07)	1.09(−05)	1.01(−05)	1.96(−11)	1.79(−11)
6.0	1.10(−05)	1.02(−05)	2.54(−07)	2.46(−07)	1.07(−05)	9.49(−06)	1.84(−11)	1.68(−11)
8.0	9.74(−06)	7.72(−06)	1.31(−07)	1.15(−07)	1.09(−05)	9.47(−06)	1.88(−11)	1.64(−11)
10.0	1.05(−05)	8.33(−06)	8.06(−08)	6.57(−08)	1.12(−05)	9.78(−06)	1.99(−11)	1.67(−11)

equations, and to check the self-consistency of the two different DAF approaches to the Fokker–Planck equation, we consider the bistable system,

$$\frac{\partial f(x,t)}{\partial t} = -\frac{\partial}{\partial x}(\gamma x - g x^3) f(x,t) + \epsilon \frac{\partial^2}{\partial x^2} f(x,t). \quad (22)$$

The Langevin's equation corresponding to Eq. (22) describes a system undergoing nonlinear Brownian motion,

$$\frac{\partial}{\partial t} x(t) = \gamma x(t) - g x^3(t) + F(t), \quad (23)$$

where $F(t)$ is a time-dependent fluctuating force satisfying the Gaussian white noise relation,

$$\langle F(t) | F(t') \rangle = 2\epsilon \delta(t-t'). \quad (24)$$

Here the parameters $\gamma = g = 1$ and $\epsilon = 0.0125$ are chosen for the present computation.

This equation has received a lot of attention in the literature. An analytical treatment of this system was reported by van Kampen and Dekker.[31] A scaling theory analysis of this model was given by Suzuki.[13] A formal analysis from a chemical kinetic point of view was presented by Larson and Kostin.[32] Indira *et al.*[26] obtained a numerical solution for the system using both finite-element and Monte Carlo methods. Blackmore and Shizgal[16] calculated the first 25 eigenvalues of this system for a few ϵ values.

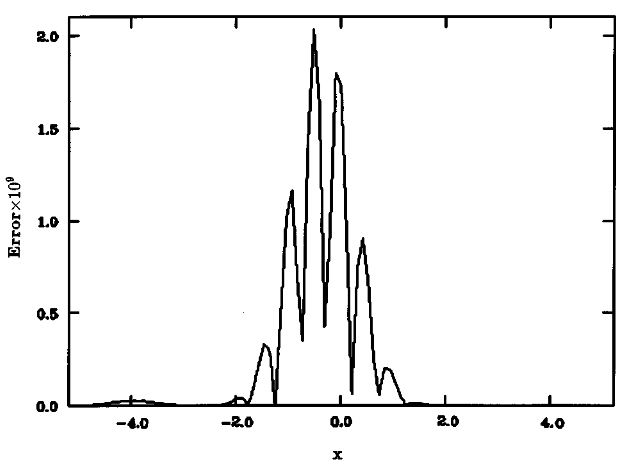

FIG. 4. The pointwise errors of the solution $f(x,1.0)$ for the Orstein–Uhlenbeck process ($N=100$, $\Delta t=0.01$, $R=4$).

A detailed numerical study of the bistable system, via an eigenfunction (obtained using the DAF form of the relevant operator) expansion approach, was pursued in our earlier paper[17] for a variety of ϵ values, including ones that had not been considered previously by other methods. It was found that the DAF eigenfunction approach achieves the same level of accuracy as Shizgal's method while requiring a smaller number of grid points. We refer the reader to the our earlier paper[17] for more details. In the present work both the DAF-eigenfunction expansion and the time-dependent DAF propagation treatment are applied and two sets of solutions are compared. The former has been described in our previous paper. The first 20 eigenvalues, calculated by using 60 grid points ($N=60$) on a sufficient large interval of $[-1.44,1.44]$, are presented in Table III for $\epsilon=0.0125$. The time-dependent DAF solutions are calculated using 60 grid points ($N=60$) and the fourth-order approximation ($R=4$) with $\Delta t=0.01$. The initial distribution is chosen as $f(x,t_0) = \delta(x)$. The time evolution of the initial delta distribution is plotted in Fig. 5. The reliability and consistency of the DAF-based approaches are tested by comparing two sets of solutions, one obtained from the eigenfunction expansion and the other from the time-dependent propagation method. As shown in Table IV, the two sets of solutions agree pointwise up to six significant figures, while using only 60 grid points!

TABLE III. Eigenvalues for the bistable system ($\epsilon=0.0125$).

λ_1	0.91(−09)	λ_{11}	4.307 333
λ_2	0.958 973	λ_{12}	4.771 923
λ_3	1.816 020	λ_{13}	5.283 940
λ_4	1.825 073	λ_{14}	5.834 524
λ_5	1.834 637	λ_{15}	6.418 896
λ_6	2.560 753	λ_{16}	7.036 294
λ_7	3.007 311	λ_{17}	7.685 715
λ_8	3.163 163	λ_{18}	8.366 050
λ_9	3.424 569	λ_{19}	9.076 368
λ_{10}	3.868 580	λ_{20}	9.815 860

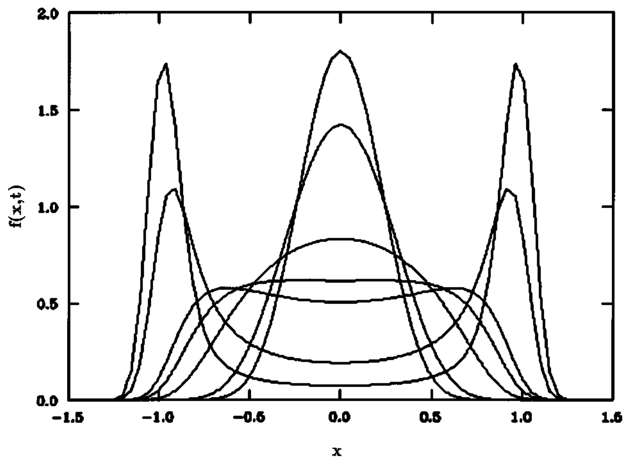

FIG. 5. The numerical solutions ($N=60$, $\Delta t=0.01$, $R=4$) of the bistable system ($\epsilon=0.0125$). The centerlines in the descending order are at $t=0.8;1.0;1.5;1.8;2.0;3.0;4.0$. The initial delta distribution is at $x=0.0$.

Obviously no graphical difference can be observed between the two different DAF solutions. We note that the present results are also graphically identical with those obtained by Shizgal's method.[16] For very short times the solutions are dominated by the largest eigenvalues. With an increase in time, the lower eigenvalues begin to contribute and eventually only the zero eigenvalue state (the ''nonpropagating'' state) contributes. A comparison of eigenfunction expansion results with those of Suzuki's scaling theory[13] was given by Blackmore and Shizgal.[16] Basically, the scaling theory provides a good approximation only at some intermediate times.

IV. CONCLUSION

As a natural continuation of our earlier work dealing with the application of the DAF method to solve the Fokker–Planck equation numerically via an eigenfunction expansion, we have examined in this paper a DAF-based time-dependent propagation approach for solving Fokker–Planck equations. Three typical benchmark problems, which have been used as standards for testing various new numerical methods, were chosen to demonstrate further the usefulness and to test the accuracy of the present approach. In the first example, a Markovian Wiener process is considered. The Fokker–Planck equation for the Wiener process resembles the classical heat equation, and has an exact solution as a Gaussian distribution. The DAF-based time-dependent propagation performs extremely well for this system. Only 50 grid points in a large interval of $[-10,10]$ and a reasonably large time increment of $\Delta t=0.01$ were needed for the DAF computation. At $t=2.0$, the DAF L_∞ error for this system is of the order 10^{-11}!

An Ornstein–Uhlenbeck process was chosen as the second numerical example. In comparison to the Wiener process, the Ornstein–Uhlenbeck process has a linear first moment as well as a nonvanishing second moment. The corresponding Ornstein–Uhlenbeck Fokker–Planck equation describes the competition between a deterministic drift force and random fluctuations. The exact solution is a moving Gaussian distribution. The DAF-based time-dependent propagation approach was tested using a variety of grid point and time increments. In all cases the DAF solutions deliver excellent accuracy. In the cases where $N=100$, $\Delta t=0.01$, $t>2.0$ and $R=4$, the DAF approach is again accurate to no fewer than ten significant figures! These are the most accurate numerical solutions yet available for this equation, as far as we are aware.

The reliability and usefulness of the DAF method is further demonstrated by considering a bistable diffusion model. It has various physical applications, but its Fokker–Planck equation cannot be solved analytically. A DAF method for this system can be obtained in two different ways: using an eigenfunction expansion approach and using a time-dependent wave packet propagation. Remarkably, the two sets of DAF solutions, obtained by means of these two entirely different approaches, agree to no fewer than five significant figures with only 60 grid points. These three examples demonstrate again that the DAF approach is an efficient, extremely accurate, and very simple method for the solution of the linearized Fokker–Planck equation. These DAF approaches are particular reliable since the self-

TABLE IV. Solutions for the bistable system ($\epsilon=0.0125$) calculated from both the eigenfunction expansion (EFE) and the time-dependent treatment (TDT).

	Time = 0.5		Time = 1.0		Time = 2.0	
x	EFE	TDT	EFE	TDT	EFE	TDT
0.000	2.727 133	2.727 133	1.423 121	1.423 121	0.503 888	0.503 888
0.096	2.205 743	2.205 747	1.351 472	1.351 474	0.506 337	0.506 338
0.192	1.159 662	1.159 664	1.153 554	1.153 556	0.513 653	0.513 654
0.288	0.388 665	0.388 666	0.875 671	0.875 673	0.525 650	0.525 652
0.384	0.080 293	0.080 293	0.579 938	0.579 939	0.541 688	0.541 689
0.480	0.009 730	0.009 730	0.325 040	0.325 041	0.559 875	0.559 876
0.576	0.000 646	0.000 646	0.147 239	0.147 239	0.575 116	0.575 117
0.672	0.000 021	0.000 021	0.050 352	0.050 352	0.574 578	0.574 580
0.768	0.000 000	0.000 000	0.011 763	0.011 763	0.529 729	0.529 730
0.864	0.000 000	0.000 000	0.001 624	0.001 624	0.398 480	0.398 481
0.960	0.000 000	0.000 000	0.000 108	0.000 108	0.190 520	0.190 521
1.056	0.000 000	0.000 000	0.000 003	0.000 003	0.038 733	0.038 734

consistency check using the energy and time domain DAF methods can be performed for a wide class of applications. In future work we will examine the application of DAFs to the nonlinear Fokker–Planck equation[20] and multispatial variable Fokker–Planck equations. We shall also study the DAF approach to other kinetic equations such as the Boltzmannequation.

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