

Distributed approximating functional approach to the Fokker–Planck equation: Eigenfunction expansion

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The distributed approximating functional method is applied to the solution of the Fokker–Planck equations. The present approach is limited to the standard eigenfunction expansion method. Three typical examples, a Lorentz Fokker–Planck equation, a bistable diffusion model and a Henon–Heiles two-dimensional anharmonic resonating system, are considered in the present numerical testing. All results are in excellent agreement with those of established methods in the field. It is found that the distributed approximating functional method yields the accuracy of a spectral method but with a local method's simplicity and flexibility for the eigenvalue problems arising from the Fokker–Planck equations. © 1997 American Institute of Physics. [S0021-9606(97)50612-X]

I. INTRODUCTION

The Fokker–Planck equation (FPE) is one of the most important kinetic equations, and accordingly has received a great deal of theoretical attention in recent years^{1–14} because it is capable of describing a broad range of scientific phenomena, such as the relation of fluctuations to the random force, and nonlinearity in pattern formation. Many chemical, biological and physical systems can be described by the Fokker–Planck equation with nonlinear coefficients. In particular, cooperative phenomena can also be modeled by FPEs. The Fokker–Planck equation is important also because its connections to other well known kinetic equations¹⁵ such as Boltzmann's equation, Landau's equation, master equations, Kramers' equation and Langevin's equation, to name only a few. The relaxation toward equilibrium of many macroscopic systems that are far from thermodynamic equilibrium can be well represented by the Fokker–Planck equation.

Analytic solutions to an appropriate kinetic equation have often proved to be essential to the conceptual understanding of the behavior of a dynamical system. Unfortunately, as in the cases of other kinetic equations, the analytical solutions to the Fokker–Planck equations are limited to only a few simple systems. Numerical approaches to solutions are indispensable for more general and complicated problems. A variety of different numerical methods have been considered for the FPE. As one may expect, each of the proposed methods has its advantages and limitations. Due to the formal similarities of the Fokker–Planck equation and the Schrödinger equation, an eigenfunction expansion method, analogous to a bound state expansion treatment of the Schrödinger equation, is very useful for the Fokker–

Planck equation. In particular, in cases like a bistable system, the full set of eigenfunctions and eigenvalues determines completely the dynamics of the Fokker–Planck equation. In order to obtain an accurate description of the time evolution of the probability distribution, a high precision evaluation of the eigenvalues is important for the detailed dynamics governed by the Fokker–Planck equation, in particular for the short time behavior. Of course, there are some essential differences between the physical significance of the Schrödinger equation and the Fokker–Planck equation. The Schrödinger equation is exact for a closed system and its eigenvalues are experimentally measurable. In contrast, the Fokker–Planck equation is an approximation describing the behaviour of a large (open) system. Therefore, asymptotic approximation methods, such as is provided by WKB analysis,⁴ can play a special role in studies of the long time behavior of the system. An interesting aspect associated with the long time behavior is the occurrence of exponentially small eigenvalues, which can be very accurately determined by the WKB method.⁴ However, accurate numerical solutions can play a complementary role to that of the analytical approximations. Shizgal¹⁶ has proposed an interesting spectral method which utilizes nonclassical weight functions and solves the FPE by an eigenfunction expansion formalism. This method is accurate and rapid in convergence.^{16,10} The goal of the present paper is to apply the recently developed distributed approximating functional (DAF) method^{18,19} to the solutions of the nonlinear coefficient FPEs. The DAF method can be applied to the Fokker–Planck equation in a variety of different ways. Two possible approaches are the eigenfunction expansion and a direct time-dependent treatment. In the present paper we focus on the eigenfunction expansion since DAFs have been applied previously to the similar eigenvalue problem for the Schrödinger equation.²⁰ Specifically, the present work considers the typical Fokker–Planck equation of the form

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$$\frac{\partial f(x,t)}{\partial t} = \frac{\partial[A(x)f(x,t)]}{\partial x} + \frac{\partial^2[B(x)f(x,t)]}{\partial x^2}, \quad (1)$$

where the drift coefficient $A(x)$ and the diffusion coefficient $B(x)$ can be nonlinear in the variable x . The quantity $f(x,t)$ is the probability distribution function satisfying Eq. (1). The present results, which are in terms of an eigenfunction expansion, are compared with those of other established methods in the field, in particular with that of Shizgal's method.^{10,21} It is found that DAF approach can provide an equivalent order of accuracy to previous spectral methods using a similar number of grid points. However, the DAF method is considerably simpler than Shizgal's approach.^{16,10}

This paper is organized as follows: The formalisms of both the Fokker–Planck equation and DAFs are reviewed in Section II. The theory of the Fokker–Planck equation has been extensively developed in the last few decades. The formalism of the eigenfunction expansion of the Fokker–Planck equation also has been discussed by a number of authors. We select only those details that are most relevant for our purposes. It should be noted that there is an on-going, intensive effort devoted to further theoretical development of DAFs. For the purpose of this presentation, we review only the particular DAF formalism namely the Hermite DAF which has been used throughout this work. In Section III we report results for three numerical examples. The first case is the Lorentz gas problem,^{22,23} a standard Fokker–Planck equation example. The Lorentz gas models the motion of a light particle in a heat bath of heavy particles, undergoing hard sphere collisions. The Fokker–Planck equation which governs the distribution function of the light particle is important theoretically because it can be derived either from the corresponding Boltzmann's equation or from the generalized master equation. In contrast to another important hard sphere model, the Rayleigh gas problem,²² the Lorentz gas problem cannot be solved analytically. The application of the Lorentz gas model to thermalization of electrons in a gaseous matrix has been studied.²³ The second example deals with the numerical solution of a bistable system which can physically describe the rate of transition between different sections of a potential well and has a variety of applications, including molecular dynamics and laser systems.^{1,3,4,7,9} A bistable potential can also be inverted to construct a metastable system describing Kramers' escape rate over the potential barrier. Finally, the usefulness of the DAF approach for the chaotic system is tested on a Henon–Heiles potential system.^{24,25} The Henon–Heiles potential is an important model in ergodic theory and has been used as a standard example for testing different numerical methods.^{26–29} It appears that for this problem the most accurate numerical solutions to date are those given by Shizgal and Chen.²¹ We find that the DAF results are in almost complete agreement with those given by Shizgal *et al.* In the paper, we end with a brief conclusion.

II. THEORETICAL BACKGROUND

The theory of the Fokker–Planck equation has a relatively long history starting from the early work by Einstein,³⁰

Langevin,³¹ Fokker,³² and Planck,³³ as well as many others.^{34–36} The modern theory of the Fokker–Planck equation is very rich in its content due to rapid development in analytical and computational analyses and a broad spectrum of applications. Both the theory and the history are too long to treat here, and there are excellent review papers³⁵ and monographs on the topic.^{15,37,38} However it is useful to review the part that is most relevant to the present work, namely the eigenfunction expansion method for the Fokker–Planck equation. This is given in Sec. II A. Sec. II B is devoted to the formalism of DAFs. The DAFs have been introduced^{18,19} as a computational tool for a variety of physical and chemistry problems such as solving both time-dependent and time-independent Schrödinger equations for discrete eigenvalues and scattering solutions, and for analytically fitting finite, discrete sets of potential surface data. Various forms of DAFs have been proposed for different application needs.^{39–47} A systematic review of the various realizations of DAFs for different applications is beyond the objective of the present paper. Our discussion is limited to the Hermite DAF, which is the form utilized in the present work.

A. The eigenfunction expansion of the Fokker–Planck equation

The Fokker–Planck equation (1) is a second order linear partial differential equation of the parabolic type. It is convenient to rewrite Eq. (1) as

$$\frac{\partial f(x,t)}{\partial t} = L_{FP}f(x,t), \quad (2)$$

having the formal solution

$$f(x,t) = e^{L_{FP}(t-t_0)}f(x,t_0), \quad (3)$$

where the Fokker–Planck operator L_{FP} is given by

$$L_{FP}f(x,t) \equiv \frac{\partial[A(x)f(x,t)]}{\partial x} + \frac{\partial^2[B(x)f(x,t)]}{\partial x^2}. \quad (4)$$

The quantity $f(x,t_0)$ is an initial distribution function at time t_0 .

The stationary solution of Eq. (1) is particularly important and can be expressed as

$$f_{st}(x) = C \exp\left(-\int_0^x \frac{A(y)}{B(y)} dy - \ln[B(x)]\right), \quad (5)$$

where C is a normalization factor such that

$$\int_{-\infty}^{\infty} f_{st}(x) dx = 1. \quad (6)$$

We adopt natural boundary conditions [such that $f(\pm\infty, t) = 0$] in the present work. In the eigenfunction expansion method it is assumed that the Fokker–Planck operator has a discrete spectrum,

$$L_{FP}f_n(x) = -\lambda_n f_n(x), \quad (7)$$

where the eigenfunctions $f_n(x)$ form a biorthogonal basis such that the *initial* probability distribution function $f(x, t_0)$ can be expressed as

$$f(x, t_0) = \sum_n a_n f_n(x, t_0), \quad (8)$$

where the coefficients a_n are determined by

$$a_n = \int_{-\infty}^{\infty} f_n(x, t_0) f(x, t_0) [f_0(x, t_0)]^{-1} dx, \quad (9)$$

with $f_0(x, t_0) \equiv f_0(x)$ being the equilibrium distribution. In its eigenfunction expansion, the full solution, Eq. (3) of the Fokker–Planck equation, is written as

$$f(x, t) = \sum_n a_n \exp[-\lambda_n(t - t_0)] f_n(x, t_0). \quad (10)$$

Equation (10) has been intensively discussed by various authors. Since the Fokker–Planck operator L_{FP} is in general *not* a Hermitian operator, it may have various types of spectra that govern the dynamical evolution of the physical system under study. In this work the existence of an equilibrium distribution for sufficiently large time is assumed. Therefore the eigenvalues λ_n are positive semidefinite:

$$\begin{aligned} \lambda_0 &= 0, \\ \lambda_n &> 0, \quad \forall n > 0. \end{aligned} \quad (11)$$

By analogy to Bloch's equation for a spin system, the inverse $1/\lambda_n$ of the eigenvalue is a fundamental relaxation time of the system. In the eigenvalue problem, it is more convenient to work with a self-adjoint operator. In order to construct a self-adjoint Fokker–Planck operator, let us consider a particular case of Eq. (5),

$$f_0(x) = \frac{1}{B(x)} \exp\left(-\int_0^x \frac{A(y)}{B(y)} dy\right). \quad (12)$$

By separating $f_0(x)$ from Eq. (2), one can obtain a new equation,

$$\begin{aligned} \frac{\partial \Phi(x, t)}{\partial t} &= -A(x) \frac{\partial \Phi(x, t)}{\partial x} + B(x) \frac{\partial^2 \Phi(x, t)}{\partial x^2} \\ &= -L\Phi(x, t), \end{aligned} \quad (13)$$

where $\Phi(x, t)$ is defined by

$$f(x, t) = f_0(x) \Phi(x, t). \quad (14)$$

The quantity $\Phi(x, t)$ can be expanded by a complete set of eigenfunctions for the operator L in Eq. (13) according to

$$\Phi(x, t) = e^{-L(t-t_0)} \Phi(x, t_0) = \sum_n b_n e^{-\varepsilon_n(t-t_0)} \phi_n(x), \quad (15)$$

where the associated eigenvalue equation is

$$L\phi_n(x) = \varepsilon_n \phi_n(x). \quad (16)$$

The expansion coefficient b_n is determined also by the initial condition $f(x, t_0)$. The Fokker–Planck operator, L , is a self-adjoint operator on the space spanned by basic functions

ϕ_n with the inner product defined with respect to the weight function $f_0(x)$. The Fokker–Planck eigenvalue problem (16) can be solved directly by numerical methods. In order to make a direct comparison between the present results and those in literature, we rewrite the Fokker–Planck equation in the form of a Schrödinger equation:

$$-\frac{\partial^2 \psi_n(z)}{\partial z^2} + V(z) \psi_n(z) = \varepsilon_n \psi_n(z), \quad (17)$$

where $\psi_n(z)$ is given by

$$\psi_n(z) = (f_0[x(z)] \sqrt{B[x(z)]})^{1/2} \phi_n[x(z)], \quad (18)$$

and the functional relation between x and z is

$$z(x) = \int^x [B(y)]^{-1/2} dy. \quad (19)$$

The effective potential V is known as a ‘‘supersymmetric potential,’’ which arises in the supersymmetric quantum mechanics,^{48,49}

$$V(z) = \frac{1}{4} [W^2(z) - 2W'_z(z)], \quad (20)$$

where the function $W(z)$ can be obtained from the general drift and diffusion functions as

$$W(z) = \frac{1}{\sqrt{B[x(z)]}} \left(A[x(z)] + \frac{1}{2} B'_x[x(z)] \right). \quad (21)$$

This similarity between the self-adjoint Fokker–Planck operator and the Schrödinger operator is the major inspiration of the present work because the previous studies²⁰ indicate that the DAF-based methods are extremely powerful for treating the quantum dynamics and the eigenvalues of the Schrödinger operator. The relevant details of the DAF are summarized in the next subsection.

B. Method of distributed approximating functionals

The distributed approximating functionals (DAFs) have been introduced^{18,19} as a mapping of a certain set of continuous L^2 -functions, called the DAF-class of functions, to itself, accurate to a given tolerance. It can be formulated so that the mapping samples the function of interest only on a discrete set of points. The range of the mapping has the property (in the so called ‘‘well tempered’’ regime) of providing the same order accuracy for derivatives of the function, as for the function itself. The continuous mapping in the Hermite DAF case is *always* well tempered (The DAF-mapping is *exact* for polynomials with degree $M+1$, where M is the degree of polynomials being used for constructing the DAF. Polynomials, of course, are *not* L^2 .) The ability of DAF to provide an analytical representation of a function and its derivatives in terms of a discrete set of values of the function only is the key for its successful usage in various computational applications. Various realizations of DAFs have been proposed depending on the different needs in the applications. We limit the following discussion to the Hermite DAF, which is the form utilized exclusively in the present work.

It is well known that a delta functional $\delta(x-x')$ has properties such that

$$f(x) = \int_{-\infty}^{\infty} \delta(x-x') f(x') dx' \quad (22)$$

$$f^{(l)}(x) = \int_{-\infty}^{\infty} \delta^{(l)}(x-x') f(x') dx', \quad (23)$$

where we assume the function $f(x)$ and its derivative $f^{(l)}$ vanish on the boundary. However relations (22)–(23) are of little numerical utility for practical computations; e.g., they cannot be directly approximated by quadrature. An approximation to the delta functional is constructed by using the usual even Hermite polynomials H_{2n} as

$$\delta_M(x-x') = \frac{1}{\sigma} \exp\left(\frac{-(x-x')^2}{2\sigma^2}\right) \times \sum_{n=0}^{M/2} \left(\frac{-1}{4}\right)^n \frac{1}{\sqrt{2\pi n!}} H_{2n}\left(\frac{x-x'}{\sqrt{2}\sigma}\right). \quad (24)$$

Obviously for a finite σ the Hermite DAF $\delta_M(x-x')$ becomes identical to the delta functional when the degree of polynomial M goes to infinity,

$$\lim_{M \rightarrow \infty} \delta_M(x-x') = \delta(x-x'). \quad (25)$$

Additionally, for fixed M , the Hermite DAF becomes identical to $\delta(x-x')$ in the limit $\sigma \rightarrow 0$. Computationally, the Hermite DAF, Eq. (24), can be discretized by quadrature. With an appropriate choice of M and σ , the Hermite DAF provides a controllable approximation to appropriate functions on a grid point,

$$f(x_j) \approx f_M(x_j) = \Delta \sum_l \delta_M(x_j - x_l) f(x_l), \quad (26)$$

where Δ is the grid spacing. Moreover, the derivatives of the Hermite DAF provide an approximation to $d^l[\delta(x-x')]/dx$, and therefore can be used to generate derivatives of the DAF-class of functions. They are called “differentiating DAFs,” and can be worked out analytically as

$$\begin{aligned} \delta_M^{(l)}(x-x') &\equiv \frac{d^l}{dx^l} \delta_M(x-x') \\ &= \frac{2^{-l/2}}{\sigma^{l+1}} \exp\left(\frac{-(x-x')^2}{2\sigma^2}\right) \sum_{n=0}^{M/2} \left(\frac{-1}{4}\right)^n \\ &\quad \times (-1)^l \frac{1}{\sqrt{2\pi n!}} H_{2n+l}\left(\frac{x-x'}{\sqrt{2}\sigma}\right). \end{aligned} \quad (27)$$

Equation (27), together with Eq. (23), implies that a differentiation has been converted into an algebraic operation in the DAF representation. This important feature makes the DAFs a powerful computational tool for solving various ordinary and partial differential equations. In particular, the Hermite DAF representation of the self-adjoint Fokker–Planck operator L is

$$\begin{aligned} L(x_i, x_j) &= \Delta A(x_i) \frac{1}{\sqrt{2}\sigma^2} \exp\left(\frac{-(x_i-x_j)^2}{2\sigma^2}\right) \\ &\quad \times \sum_{n=0}^{M/2} \left(\frac{-1}{4}\right)^n (-1) \frac{1}{\sqrt{2\pi n!}} H_{2n+1}\left(\frac{x_i-x_j}{\sqrt{2}\sigma}\right) \\ &\quad + \Delta B(x_i) \frac{1}{\sqrt{2}\sigma^3} \exp\left(\frac{-(x_i-x_j)^2}{2\sigma^2}\right) \\ &\quad \times \sum_{n=0}^{M/2} \left(\frac{-1}{4}\right)^n \frac{1}{\sqrt{2\pi n!}} H_{2n+2}\left(\frac{x_i-x_j}{\sqrt{2}\sigma}\right). \end{aligned} \quad (28)$$

This form can be used directly for numerical diagonalization. For simplicity, we have restricted our discussion to the one-dimensional case. A systematic generalization to two or more dimensions is straightforward.

The most attractive properties of the Hermite DAF for solving differential equations are the following: (i) It transforms the ordinary and partial differentiations into algebraic calculations. This implies that the Hermite DAF can provide the same level of accuracy as that of spectral methods. (ii) The global nature of the spectral methods makes their practical applications for complicated boundary condition and complex geometry problems difficult. By contrast, the Hermite DAF leads to a local method. This property endows the Hermite DAF with sufficient flexibility to handle complicated boundary conditions and geometries. In particular, since the DAF does not require a Gaussian or fixed sampling quadrature rule in its discretization, the number of grid points is not tied to the degree of the polynomial. This implies that DAFs can be used for an arbitrarily large domain without introducing a large number of basis functions. (iii) Furthermore, the matrix elements of the DAF representation of a differential operator is highly banded. The bandedness of the DAF matrices can be incorporated in the necessary matrix-vector operations so as to dramatically speed up the computation and thereby reduce the computation cost.

As demonstrated in the next section, the DAF is a simple and reliable method for the eigenvalue class of problems described by the Fokker–Planck equations. It provides a similar level of accuracy and speed of convergence as that characteristic of spectral methods.

III. NUMERICAL APPLICATIONS

In order to demonstrate the usefulness, test the accuracy and explore the limitations of the DAF method for the Fokker–Planck equations, three “standard” problems are considered. The results for these are compared with those obtained by other authors using various methods. The details of the present study are given in the following three subsections. In the present computation, the Hermite DAF parameters are taken as $M=88$ and $\sigma=3.05\Delta$ for all examples.

A. Lorentz gas

As the first example we consider a hard sphere collision Lorentz gas problem. The corresponding self-adjoint Fokker–Planck operator L for this problem is

TABLE I. Eigenvalues of the Lorentz Fokker–Planck operator.

	ϵ_1	ϵ_2	ϵ_3	ϵ_6	ϵ_{10}
Shizgal <i>et al.</i>	4.683 40	10.112 52	16.429 68	40.052 38	80.447 94
Present	4.683 40	10.112 52	16.429 68	40.052 38	80.447 94
	ϵ_{15}	ϵ_{20}	ϵ_{30}	ϵ_{40}	
Shizgal <i>et al.</i>	142.4461	215.1631	387.623	590.867	
Present	142.4461	215.1630	387.620	590.858	

$$L = A(x) \frac{\partial}{\partial x} - B(x) \frac{\partial^2}{\partial x^2} = (2x^2 - 3) \frac{\partial}{\partial x} - x \frac{\partial^2}{\partial x^2}. \quad (29)$$

The effective potential $V(z)$, Eq. (20), is

$$V(z) = \frac{z^6}{64} - z^2 + \frac{15}{4z^2}. \quad (30)$$

[Note the functional relation between z and x is given by Eq. (19)]. This potential has singularities both at zero and at infinity. This eigenvalue problem has been considered by a number of authors, using various methods, such as the Sonine polynomial expansion,^{23,50} the Wigner–Wilkins kernel⁵¹ and the Rayleigh–Ritz variational procedure.^{52,53} Shizgal and Chen²¹ recently reported an accurate calculation employing a nonclassic weight function $w(z) = z^5 \exp(-z^4/16)$. They obtained very rapid convergence with the first 40 eigenvalues accurately calculated using 70 or fewer grid points. The physical domain of definition for the problem is $[0, \infty)$. As indicated by Shizgal and Chen, the computing interval has to be sufficiently large in order for the large eigenvalues to be convergent. The results for the first 40 eigenvalues, using 70 grid points in z are found to be in excellent agreement with those given by Shizgal and Chen; detailed results for the DAF approach, as compared to those of Shizgal and Chen are listed in Table I.

B. A bistable system

To demonstrate further the reliability and robustness of the DAF method for the Fokker–Planck equations, the equation describing a typical bistable system is considered:

$$\frac{\partial f(x,t)}{\partial t} = -\frac{\partial}{\partial x}(\gamma x - gx^3)f(x,t) + \epsilon \frac{\partial^2}{\partial x^2} f(x,t). \quad (31)$$

Here the parameters γ , g and ϵ are positive and are related to one another through the fluctuation-dissipation theorem at equilibrium. In the case of a system far from equilibrium, γ , g , and ϵ become independent of each other. We set $\gamma = g = 1$ for simplicity in the present work. This equation has received a lot of attention in the literature. An analytical approach to this system was reported by van Kampen, Dekker and van Kampen.¹ Suzuki used this system as a model for testing scaling theory.³ Caroli *et al.* presented a powerful systematic WKB treatment for this system.⁴ They showed that the final approach to equilibrium is governed by the Kramers high-viscosity rate. They also point out the validity and limitation of Suzuki's scaling theory for this system.

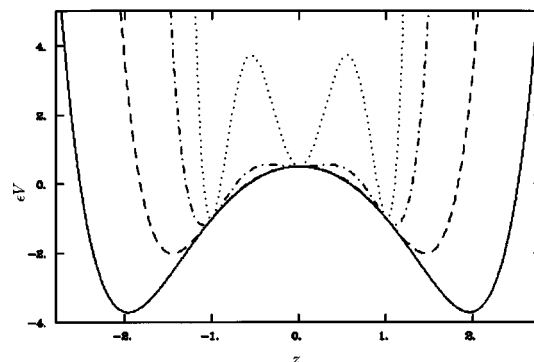


FIG. 1. Scaled potential $[\epsilon V(z)]$ of the bistable system, Eq. (32); solid line: $\epsilon = 5$; dashed line: $\epsilon = 1$; dash-dotted line: $\epsilon = 0.1$; dotted line: $\epsilon = 0.01$.

Larson and Kostin⁶ reported a formal analysis from a chemical kinetic point of view. Indira *et al.*⁷ obtained a numerical solution for the system using both finite-element and Monte Carlo methods. Shizgal's method has also been applied to the system to calculate accurately the first 25 eigenvalues.

The corresponding effective potential for Eq. (31) is

$$V(z) = \frac{(z^3 - z)^2}{4\epsilon^2} - \frac{1}{2\epsilon}(3z^2 - 1), \quad (32)$$

where the size of ϵ determines the physical regime described in the problem. The scaled potential $[\epsilon V(z)]$ is pictured in Fig. 1. For ϵ sufficiently small, one has a triple well potential which supports three isolated, approximately harmonic systems at low energy. For intermediate ϵ , the potential has three shallow wells coupled to each other with the three minima at the points

$$z = 0, \quad \pm \left[\frac{2}{3} + \left(\frac{1}{9} + 2\epsilon \right)^{1/2} \right]^{1/2}. \quad (33)$$

For sufficiently large ϵ , the potential transforms into a double well type with a maximum at the origin and two minima at $z = \pm \left[\frac{2}{3} + \left(\frac{1}{9} + 2\epsilon \right)^{1/2} \right]^{1/2}$. The potential asymptoti-

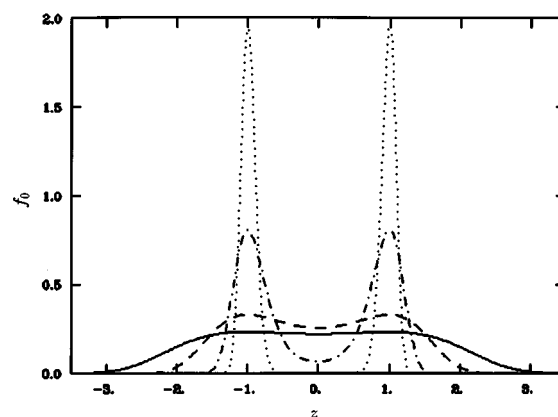


FIG. 2. Equilibrium distribution functions for the bistable system; solid line: $\epsilon = 5$; dashed line: $\epsilon = 1$; dash-dotted line: $\epsilon = 0.1$; dotted line: $\epsilon = 0.02$.

TABLE II. Eigenvalues of the Fokker–Planck operator for a bistable system ($\epsilon=0.1$).

	Shizgal <i>et al.</i> ($N=60$)	Present ($N=50$)	Present ($N=60$)	Present ($N=300$)
λ_1	3.354 5300(−02)	3.354 5287(−02)	3.354 5287(−02)	3.354 5287(−02)
λ_2	0.927 372	0.927 372	0.927 372	0.927 372
λ_3	1.680 264	1.680 264	1.680 264	1.680 264
λ_5	3.733 985	3.733 985	3.733 985	3.733 985
λ_{10}	11.687 442	11.687 441	11.687 441	11.687 441
λ_{15}	22.639 908	22.639 909	22.639 909	22.639 909
λ_{20}	36.031 815	36.031 788	36.031 787	36.031 787
λ_{25}	51.5419	51.5361	51.5360	51.5360

cally behaves as z^6 and obviously supports infinity many discrete states. The stationary solutions for various ϵ values are plotted in Fig. 2.

Blackmore and Shizgal¹⁰ reported the numerical calculation of eigenvalues for the parameter values $\epsilon=0.1, 0.01$, respectively, and given a detailed numerical analysis for various physical behaviors of the system for small ϵ ($\epsilon=0.1, 0.01$). In the present work, we perform eigenvalue calculations for $\epsilon=0.1, 0.01$ using the Hermite DAF. For convenience of comparison, all eigenvalues in this subsection are measured in units of ϵ (so $\lambda_n = \epsilon \epsilon_n$). As listed in Table II, for $\epsilon=0.1$ the DAF calculation is already convergent using only 50 grid points, yielding the first 25 eigenvalues that are in very good agreement with the results obtained by Shizgal's method using up to 60 grid points. The DAF results for the first 25 eigenvalues for $\epsilon=0.01$ is listed in Table III. Except for the first excited state, all eigenvalues are converged up to 6 significant figures using only 60 grid points. Similar calculations by Blackmore and Shizgal with 100 grid points are also included in Table III for reference. As noted by Blackmore and Shizgal, the first few excited states converge more slowly as ϵ decreases. This tendency becomes stronger for $\epsilon=0.001$. This is because the first few eigenvalues approach zero as $\epsilon \rightarrow 0$ and the corresponding eigenfunctions are confined by the potential barriers at the bottoms of the wells and are sensitive to the shape of the potential in these regimes (see Fig. 3). The higher energy eigenstates exhibit the typical global behavior. However, these large eigenvalues generally converge more slowly and require more grid points for smaller ϵ values. A test calculation for $\epsilon=0.0001$ indicates that significantly more grid points are needed to converge the first 50 eigenvalues. It is

noted that the analytic approximation methods, such as the WKB approach discussed by Caroli *et al.*,⁴ become asymptotically accurate at the limit $\epsilon \rightarrow 0$.

The present investigation also extends to the large ϵ regime. The results of first 25 eigenvalues for $\epsilon=1, 10$ are given in Table IV. It is seen that the deep double wells have little influence on the eigenfunctions, since the lowest eigenvalues are no longer close to the bottoms of the potential wells. In such a case the system is quickly dominated by the equilibrium distribution due to the rapid diffusion. This will be the case for systems with a relatively small dimension at high temperature. The fifth eigenfunction for various ϵ ($0.001 \leq \epsilon \leq 10$) is plotted in Fig. 4. This eigenfunction exhibits the typical global behavior expected at large ϵ . The eigenfunction becomes more and more confined in the potential well regions as the value of ϵ decreases. The system begins behaving like three isolated wells when ϵ becomes smaller than 0.01. At the limit of $\epsilon \rightarrow 0$, the lowest eigenvalues approach integers with a three fold degeneracy. The eigenvalues belonging to the central well are rapidly convergent. However, those eigenvalues belonging to the left well or right well are more sensitive to the number of grid points and the range of the interval employed in the computation.

C. The Henon–Heiles potential system

The anharmonic Henon–Heiles potential^{24,25} is a chaotic model system (classically) describing a resonating system and providing a simple example for the study of Poincare surfaces and trajectories. The system is also important in numerical analysis. Various numerical methods, such as the symmetric split operator-FFT method,²⁹ Shizgal's method,²¹

TABLE III. Eigenvalues of the Fokker–Planck operator for a bistable system ($\epsilon=0.01$).

	Shizgal <i>et al.</i> ($N=100$)	Present ($N=60$)	Present ($N=100$)	Present ($N=300$)
λ_1	6.154 649 7(−12)	3.381 989 2(−11)	6.364 985 6(−12)	6.382 725 5(−12)
λ_2	0.967 865	0.967 864	0.967 864	0.967 864
λ_3	1.864 542	1.864 542	1.864 542	1.864 542
λ_5	1.866 975	1.866 975	1.866 975	1.866 975
λ_{10}	3.943 531	3.943 531	3.943 531	3.943 531
λ_{15}	5.960 839	5.960 839	5.960 839	5.960 839
λ_{20}	8.793 163	8.793 146	8.793 146	8.793 146
λ_{25}	12.2693	12.268 706	12.268 703	12.268 703

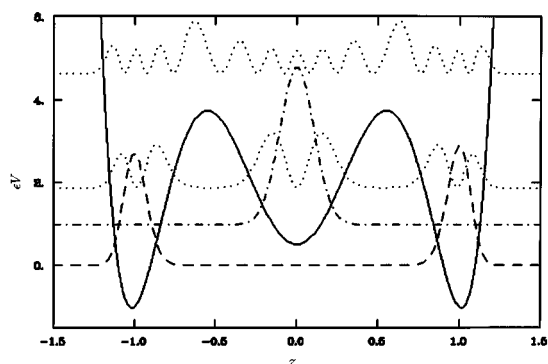


FIG. 3. Potential and ψ_n^2 of the bistable system ($\epsilon=0.01$); solid line: the potential; dashed line: $n=1$; dash-dotted line: $n=2$; lower dotted line: $n=3$; upper dotted line: $n=12$.

the semiclassical method and a quantum mechanical Hermite basis set expansion method^{26,27} have been tested on the Henon–Heiles potential. A preliminary study, based on the Hermite DAF method, has been carried out using the formalism of the spectral density operator and Chebychev expansion.²⁰ The purpose of the present calculation is to demonstrate the accuracy and the speed of convergence of the DAF approach for two-dimensional systems in statistical mechanics.

The Schrödinger-like Fokker–Planck equation (17) for this system is given by

$$\left[-\frac{1}{2} \frac{\partial^2}{\partial x^2} - \frac{1}{2} \frac{\partial^2}{\partial y^2} + \frac{1}{2} x^2 + \frac{1}{2} y^2 - \lambda x \left(\frac{1}{3} x^2 - y^2 \right) \right] \phi_{nm}(x, y) = \epsilon_{nm} \phi_{nm}(x, y), \quad (34)$$

where the principal quantum number n and angular momentum quantum number m have been discussed by Noid and Marcus.²⁶ Obviously the parameter λ is a measure of the anharmonicity of the two-dimensional system and is here taken to be $\sqrt{0.0125}$ to enable the comparison of our results with those of other authors. The potential has a C_{3v} symmetry, which fact has been utilized by Noid and Marcus to speed up their computation. Earlier work by Marcus *et al.*²⁷ was based on two sets of 990 and 1225 basis states, respectively. Feit *et al.*²⁹ report an accurate calculation using their split operator-FFT method, requiring 16384 time steps. A recent computation by Shizgal and Chen has achieved six significant figures of accuracy for the eigenvalues as high as $\epsilon_{13,3}$, using 50 or fewer grid points in each dimension. With the flexibility in choosing the appropriate weight function, it is not surprising that Shizgal's method can attain very rapid convergence.

The present work proceeds by first constructing the two-dimensional version of the DAF representation of the Fokker–Planck operator, Eq. (28). The eigenvalues and eigenfunctions are obtained by subsequent numerical diagonalization of the discrete DAF-Fokker–Planck operator. The present results are calculated using 50 grid points in x and 50 grid points in y (for a total of 2500 grid points). As shown in

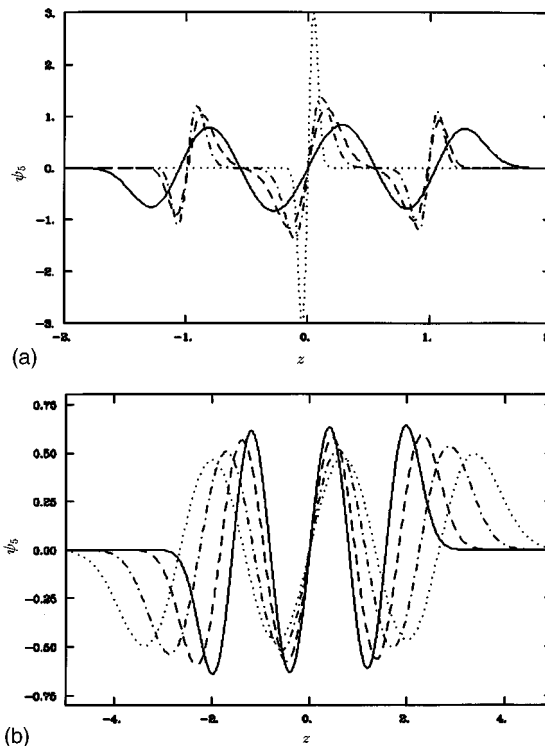


FIG. 4. (a). Eigenfunction ψ_5 of the bistable system; solid line: $\epsilon=0.1$; dashed line: $\epsilon=0.01$; dash-dotted line: $\epsilon=1/180$; dotted line: $\epsilon=0.001$. (b) Eigenfunction ψ_5 of the bistable system; solid line: $\epsilon=1$; dashed line: $\epsilon=2$; dash-dotted line: $\epsilon=2$; dotted line: $\epsilon=10$.

TABLE IV. Eigenvalues of the Fokker–Planck operator for a bistable system.

	$\epsilon=1$	$\epsilon=10$
λ_1	0.792088	3.703574
λ_2	3.548889	13.073649
λ_3	6.843548	24.583005
λ_4	10.826974	38.281305
λ_5	15.415273	53.883265
λ_6	20.539520	71.183340
λ_7	26.152861	90.033533
λ_8	32.219147	110.318967
λ_9	38.709220	131.947015
λ_{10}	45.598922	154.840940
λ_{11}	52.867811	178.935823
λ_{12}	60.498295	204.175801
λ_{13}	68.475025	230.512150
λ_{14}	76.784453	257.901874
λ_{15}	85.414509	286.306672
λ_{16}	94.354347	315.692137
λ_{17}	103.594152	346.027139
λ_{18}	113.124988	377.283335
λ_{19}	122.938671	409.434779
λ_{20}	133.027673	442.457598
λ_{21}	143.385034	476.329736
λ_{22}	154.004298	511.030728
λ_{23}	164.879456	546.541522
λ_{24}	176.004890	582.844323
λ_{25}	187.375341	619.922461

TABLE V. Eigenvalues of the Henon–Heiles potential system.

n	l	Feit <i>et al.</i>	Shizgal <i>et al.</i>	Present
3	3	3.9825	3.982417	3.982417
3	−3	3.9859	3.985761	3.985761
5	3	5.8672	5.867015	5.867015
5	−3	5.8816	5.881446	5.881446
6	6	6.9991	6.998932	6.998932
6	−6	6.9996	6.999387	6.999387
7	3	7.6979	7.697721	7.697721
7	−3	7.7371	7.736885	7.736885
8	6	8.8116	8.811327	8.811327
8	−6	8.8154	8.815188	8.815188
9	3	9.4670	9.466773	9.466773
9	−3	9.5526	9.552382	9.552382
9	9	10.0356	10.035413	10.035413
9	−9	10.0359	10.035592	10.035592
10	6	10.5727	10.572480	10.572480
10	−6	10.5907	10.590470	10.590470
11	3	11.1603	11.160258	11.160259
11	−3	11.3253	11.325231	11.325231
11	9	11.7497	11.749519	11.749519
11	−9	11.7525	11.752297	11.752297
12	6	12.3335	12.333785	12.333785
12	−6	12.2771	12.277192	12.277192
12	12	12.7474	12.748445	12.748423
12	−12	13.0310	13.032062	13.032062
13	3	13.0868	13.086873	13.086873
13	−3	13.0800	13.081196	13.081196

Table V, our DAF approach achieves the same level of accuracy and rate of convergence as was obtained in Shizgal's method.

IV. CONCLUSION

In this paper, the DAF approach has been applied to Fokker–Planck equations using an eigenfunction expansion. Three typical examples, which cover a variety of situations, are chosen to demonstrate the usefulness and to test the accuracy of the present approach. In the first example, the Lorentz Fokker–Planck equation has a quadratic drift coefficient and a nonclassical diffusion coefficient. The effective potential for the corresponding Schrödinger-like Fokker–Planck equation is singular at the origin and at infinity, describing hard sphere collisions. The DAF performs extremely well for this system. The first 40 eigenvalues converge to six significant figures, using only 70 grid points. In the second example we considered a bistable diffusion model for a variety of choice of ϵ , the parameter determining the ratio of dissipation and convection. For $\epsilon=0.1$ and 0.01 , the speed of convergence of the DAF calculation is actually faster than that reported by Shizgal *et al.*^{10,16} We also present results for two large- ϵ cases ($\epsilon=1, 10$) using 60 grid points in each case. This parameter range has not been studied before, and so no other results are available at present for comparison. The last example studied is a two-dimensional Henon–Heiles potential for an anharmonic oscillator. The DAF method converges very rapidly in this case. The first 97 eigenvalues converge to eight significant numbers using 50 grid points in each dimension. The present results are in

excellent agreement with those of other methods, such as the semiclassical method, the symmetric split operator-FFT, a Hermite basis expansion and Shizgal's method. In all examples the DAF has been shown to yield the same level of accuracy and speed of convergence as Shizgal's method for eigenvalues. An attractive feature of DAFs is that they involve a local method's simplicity and flexibility for complicated geometries and boundary conditions, and yet yield a global method's accuracy and speed of convergence. These three examples show that the DAF approach is an efficient, reliable and particularly simple method for the solution of Fokker–Planck equations. Since for a given initial state, the time evolution of the Fokker–Planck operator is completely determined when its eigenfunctions and eigenvalues are known, the DAF approach provides a practical method for the dynamics of a general class of macroscopic systems described by the Fokker–Planck equation. In future work we will examine the application of DAFs to the Fokker–Planck equation based on a direct time-dependent approach. We also shall study the nonlinear forms of the Fokker–Planck equation.

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