Numerical evaluation of path-integral solutions to Fokker-Planck equations. II. Restricted stochastic processes

M. F. Wehner and W. G. Wolfer
Fusion Engineering Program, Nuclear Engineering Department, University of Wisconsin—Madison, Madison, Wisconsin 53706
(Received 31 May 1983)

A path-integral solution is derived for processes described by nonlinear Fokker-Planck equations together with externally imposed boundary conditions. This path-integral solution is written in the form of a path sum for small time steps and contains, in addition to the conventional volume integral, a surface integral which incorporates the boundary conditions. A previously developed numerical method, based on a histogram representation of the probability distribution, is extended to a trapezoidal representation. This improved numerical approach is combined with the present path-integral formalism for restricted processes and is shown to give accurate results.

I. INTRODUCTION

The development of a theory of nonequilibrium thermodynamics has received considerable attention in the past several years. The apparent onset of ordered structures out of random or chaotic systems is a clear example of nature driven far from the equilibrium state. Such nonequilibrium systems must be supported by a continual flow of negative entropy into the system to prevent it from relaxation.[1] This is usually supplied by the presence of external forces or by some type of externally applied boundary conditions. This latter mechanism acts as a coupling between the system and the surrounding environs and is the focus of this paper.

One of the dominant mathematical models of nonequilibrium systems is provided by the nonlinear Fokker-Planck equation.[2–5] A formal solution within the natural boundaries in terms of a covariant path integral has led to interpretations of the Onsager-Machlup functional as a nonequilibrium thermodynamic potential.[6–8] Standard equilibrium thermodynamical concepts such as thermodynamic potential, entropy, and entropy production rate can thereby be extended and quantitatively defined for systems far from equilibrium.[9,10]

In these previous investigations, however, the nonequilibrium systems were modeled as unrestricted Markovian processes which require no additional boundary conditions. For many physical systems, external boundary conditions are in fact the forces which drive the system to a state far from equilibrium.

Examples of such systems described by the nonlinear Fokker-Planck equation subject to external constraints are the following: the velocity distribution of particles in a magnetically confined plasma,[11] the growth of small gas bubbles in solids,[12] the diffusion of a penetrant into a semi-infinite body of polymer,[13] the deposition of an aerosol on a surface,[14] and the nucleation and growth of defects in an irradiated material[15] to name but a few.

It is the aim of this paper to provide the means to find the time-dependent solution of the Fokker-Planck equation in the presence of external boundary conditions. In Sec. II, a formal solution to the Fokker-Planck equation subject to external boundary conditions using th Green's-function method is presented. In Sec. III, th short-time propagator, taken from the path-integral fo malism, is shown to be an appropriate Green's functio for the general nonlinear Fokker-Planck equation. In Se IV, the various types of boundary conditions and the co struction of suitable Green's functions are discussed. I Sec. V, a boundary integral technique is introduced in o der to avoid the complicated and often impossible task c developing Green's functions specific to certain types c boundaries. Also in this section, a numerical techniq introduced in a previous paper[16] is refined and generalize to include the effect of the boundary conditions. Numer cal results for some specific problems are given in Sec. V Finally, some examples utilizing Green's functions co structed to suit the boundary conditions are solved exactl in the Appendixes A and B.

II. FORMAL SOLUTION

As a starting point, consider the multidimensio Fokker-Planck operator acting on a probability distrib tion function $p(\vec{q},t)$,

$$Lp=-\frac{\partial p(\vec{q},t)}{\partial t}-\frac{\partial}{\partial q^i}[K^i(\vec{q})p(\vec{q},t)]+\frac{1}{2}\frac{\partial^2}{\partial q^i\partial q^j}[Q^{ij}(\vec{q})p(\vec{q},t)]=-\rho(\vec{q},t),\quad i,j=1,\ldots,N \tag{}$$

where ρ is a distributed source term and $\vec{q}$ is assumed lie within some N-dimensional volume V. Note that r peated indices imply summation. Also imposed on $p(\vec{q},$ are some type of boundary conditions at the surface S the volume.

The Green's function $G(\vec{q},t;\vec{q}_0,t_0)$, satisfying th Fokker-Planck equation with an impulsive point source, defined by the equation[16]

$$LG=-\delta(\vec{q}-\vec{q}_0)\delta(t-t_0)\,. \tag{2}$$

The adjoint to the Green's function satisfies the equation

$$\tilde{L}\,\tilde{G} = -\delta(\vec{q}-\vec{q}_0)\delta(t-t_0)\ , \tag{2b}$$

where the adjoint or backwards Fokker-Planck operator $\tilde{L}$ is given as

$$\tilde{L} = \frac{\partial}{\partial t} + K^i(\vec{q})\frac{\partial}{\partial q^i} + \frac{1}{2}Q^{ij}(\vec{q})\frac{\partial^2}{\partial q^i \partial q^j}\ . \tag{2c}$$

The boundary conditions on the adjoint functions are defined to be those which are adjoint to the original boundary conditions. The relationship between these two sets of conditions can be found from

$$n^i P^i(G,\tilde{G}) = 0 \tag{3a}$$

on the surface S. Here n^i is the outward normal vector and P^i is called the bilinear concomitant[17] given for the Fokker-Planck operator as

$$P^i(u,v) = uvK^i + \frac{1}{2}uQ^{ij}\frac{\partial v}{\partial q^i} - \frac{1}{2}v\frac{\partial}{\partial q^j}(Q^{ij}u)\ . \tag{3b}$$

As a consequence of this relationship for the boundary conditions imposed on the Green's function and its adjoint, the following reciprocity principle may be proven[18]:

$$G(\vec{q},t;\vec{q}_0,t_0) = \tilde{G}(\vec{q}_0,t_0;\vec{q},t)\ . \tag{4}$$

Thus G may be interpreted as describing the effect at $\vec{q}$ of a point source located at $\vec{q}_0$ while $\tilde{G}$ describes the inverse effects. Using Eq. (4), we may operate on G by $\tilde{L}_0$ to find

$$\tilde{L}_0 G(\vec{q},t;\vec{q}_0,t_0) = \frac{\partial G}{\partial t_0} + K^i(\vec{q}_0)\frac{\partial G}{\partial q_0^i} + \frac{1}{2}Q^{ij}(\vec{q}_0)\frac{\partial^2 G}{\partial q_0^i \partial q_0^j}$$

$$= -\delta(\vec{q}-\vec{q}_0)\delta(t-t_0)\ . \tag{5}$$

Replacing the variable $\vec{q}$ by $\vec{q}_0$ in Eq. (1) and integrating the quantity

$$p(\vec{q}_0,t)\tilde{L}_0 G(\vec{q},t;\vec{q}_0,t_0) - G(\vec{q},t;\vec{q}_0,t_0)L_0 p(\vec{q}_0,t_0)$$

over subscripted space and time yields

$$\int_0^t dt_0 \int_V d^N q_0 \left[p\frac{\partial G}{\partial t_0} + G\frac{\partial p}{\partial t_0} \right] + \int_0^t dt_0 \int_V d^N q_0 \left[pK^i \frac{\partial G}{\partial q_0^i} + G\frac{\partial (K^i p)}{\partial q_0^i} \right]$$

$$+ \tfrac{1}{2}\int_0^t dt_0 \int_V d^N q_0 \left[pQ^{ij}\frac{\partial^2 G}{\partial q_0^i \partial q_0^j} - G\frac{\partial^2 (Q^{ij}p)}{\partial q_0^i \partial q_0^j} \right] = \int_0^t dt_0 \int_V d^N q_0 \rho G - p(\vec{q},t)\ . \tag{6}$$

The first integral may be performed over time. The second and third integrals may be combined and written in the form

$$\int_0^t dt_0 \int_V d^N q_0 \frac{\partial}{\partial q_0^i}[P_0^i(p,G)] = \int_0^t dt_0 \oint dS_0 n_0^i P_0^i(p,G)\ ,$$

where $\vec{P}_0$ is again the bilinear concomitant defined by Eq. (3a) but $\vec{q}_0$ has replaced $\vec{q}$. Solving for the distribution function $p(q,t)$ yields

$$p(q,t) = \int_0^t dt_0 \int_V d^N q_0 \rho(q_0,t_0) G(\vec{q},t;\vec{q}_0,t_0) + \int_V d^N q_0 p(\vec{q}_0,0) G(\vec{q},t;\vec{q}_0,0)$$

$$- \int_0^t dt_0 \oint dS_0 n_0^i \left[J^i(q_0,t_0) G(\vec{q},t;\vec{q}_0,t_0) + \tfrac{1}{2}p(\vec{q}_0,t_0)Q^{ij}(\vec{q}_0)\frac{\partial G}{\partial q_0^j}(\vec{q},t;\vec{q}_0,t_0) \right]\ , \tag{7}$$

where

$$J^i(\vec{q},t) = K^i(\vec{q})p(\vec{q},t) - \frac{1}{2}\frac{\partial}{\partial q^j}[Q_{ij}(\vec{q})p(\vec{q},t)]$$

is the probability current.

Physically, the first two terms represent the effects of the volume source distribution and the initial conditions, respectively, while the third term represents the effects of the boundary conditions. Therefore, the boundary conditions may be regarded as source distributions at the surface in analogy to problems in electrostatics, fluid mechanics, etc.[17]

Because Eq. (1) is a parabolic partial differential equation, the problem would be overspecified if both the probability current $n^i J^i$, and the value of the distribution p are specified at the surface. In this case, a solution may not physically be possible. Either one or the other or a linear combination of $n^i J^i$ and p form a sufficient boundary condition to provide a unique solution to Eq. (1). Because of this, there will, in general, be unknown terms in the surface integrals of Eq. (7). Either of two approaches may remedy this shortcoming. If the boundaries are simple enough, the construction of a certain Green's function, via the superposition principle, can cause the unknown terms to vanish. Some specific examples of this technique are shown in the Appendixes.

However, in many instances, such a Green's function cannot be found. In these cases, an integral equation must be solved. Such a technique is well established in the theory of elliptic partial differential equations and is known as the boundary integral method.[19–21]

III. PATH INTEGRALS AND SHORT-TIME PROPAGATORS

Unfortunately, Green's functions satisfying Eq. (2) even without the presence of external boundary conditions can only be found for selected choices of drift and diffusion coefficients. However, the general nonlinear Fokker-Planck equation may be expanded in time and solved to order $(\Delta t)^2$. The resulting solution, although not uniquely defined due to an ambiguity in the evaluation of the Fokker-Planck coefficients,[22-24] is a Green's function valid within the singular boundaries (see Sec. IV) for short time, $\tau=t-t_0$.

For longer times the solution may be found iteratively. This is the basis of the path-integral formalism.[25,26] From this Green's function, often called the short-time propagator, other Green's functions appropriate to the boundary conditions may be constructed or a boundary integral method developed (see Secs. IV and V).

We first need to show that in the limit of infinitesimal time, the Fokker-Planck equation together with the boundary conditions are reproduced from Eq. (7) when a short-time propagator is used as the Green's function. Such a propagator function can be written in its simplest form for the infinite space, according to Dekker,[24] if one selects as the Green's function the solution to Eq. (1) assuming that the drift vector K^i and the diffusion tensor Q^{ij} are functions of the source point $\vec{q}_0$ but not the field point $\vec{q}$. $G(\vec{q},\vec{q}_0,t)$ then has the form

$$G(\vec{q},\vec{q}_0,\tau)=(2\pi\tau)^{-n/2}[\det Q^{ij}(\vec{q}_0)]^{-1/2}\exp\left[-\frac{1}{2\tau}Q_{ij}(\vec{q}_0)[q^i-q_0^i-\tau K^i(\vec{q}_0)][q^j-q_0^j-\tau K^j(\vec{q}_0)]\right],$$

where Q_{ij} is inverse of Q^{ij}.

Rewriting Eq. (7) for a short-time interval τ suggests the following form reminiscent of the path sum:

$$p(\vec{q},t+\tau)=\int_V d^Nq_0\,p(\vec{q}_0,t)G(\vec{q},\vec{q}_0,\tau)-\int_0^\tau d\tau'\oint dS_0 n_0^i\left[J^i(\vec{q}_0,t+\tau')G(\vec{q},\vec{q}_0,\tau')+\tfrac{1}{2}P(\vec{q}_0,t+\tau')Q^{ij}(\vec{q}_0)\frac{\partial G}{\partial q_0^j}(\vec{q},\vec{q}_0,\tau')\right], \tag{8}$$

where $\rho(\vec{q},t)=0$ for clarity.

To begin the proof of such a restricted path sum we subtract $p(\vec{q},t)$ from Eq. (8), multiply by an analytic but otherwise arbitrary function, $R(\vec{q})$, divide by τ and integrate over the volume in q space resulting in

$$\begin{aligned}\int_V d^Nq\,R(\vec{q})\frac{1}{\tau}[p(\vec{q},t+\tau)-p(\vec{q},t)]=&\frac{1}{\tau}\int_V d^Nq\left[\int_V d^nq_0 G(\vec{q},\vec{q}_0,\tau)p(\vec{q}_0,t)-p(\vec{q},t)\right]R(\vec{q})\\&-\frac{1}{\tau}\int_0^\tau d\tau'\int_V d^Nq\,R(\vec{q})\oint dS_0 n_0^i\left[J^i(\vec{q}_0,t+\tau')G(\vec{q},\vec{q}_0,\tau')+\tfrac{1}{2}p(\vec{q}_0,t+\tau')Q^{ij}(\vec{q}_0)\frac{\partial G}{\partial q_0^j}(\vec{q},\vec{q}_0,\tau')\right].\end{aligned} \tag{9}$$

Expanding the arbitrary function into a Taylor series about q_0 such that

$$R(\vec{q})=R(\vec{q})+\sum_{n=1}^{\infty}\frac{1}{n!}(q^k-q_0^k)\cdots(q^l-q_0^l)\frac{\partial^n R(q_0)}{\partial q_0^k\cdots\partial q_0^l}$$

and taking the limit $\tau\to 0$ yields

$$\begin{aligned}\int_V d^Nq\,R(\vec{q})\dot{p}(\vec{q},t)=&\lim_{\tau\to 0}\frac{1}{\tau}\int_V d^Nq\int_V d^Nq_0 R(\vec{q}_0)G(\vec{q},\vec{q}_0,\tau)p(\vec{q}_0,t)\\&-\lim_{\tau\to 0}\frac{1}{\tau}\int_V d^Nq\,R(\vec{q})p(\vec{q},t)+\sum_{n=1}^{\infty}\int_V d^Nq_0 A^n_{k,\ldots,l}(\vec{q}_0)p(\vec{q}_0,t)\frac{\partial^n R(\vec{q}_0)}{\partial q_0^k\cdots\partial q_0^l}\\&-\lim_{\tau\to 0}\frac{1}{\tau}\int_0^\tau d\tau'\int_V d^Nq\,R(\vec{q})\oint dS_0 n_0^i\left[J^iG+\tfrac{1}{2}pQ^{ij}\frac{\partial G}{\partial q_0^j}\right],\end{aligned} \tag{10}$$

where the nth-order transition moments are defined to be

$$A^n_{k,\ldots,l}(\vec{q}_0)=\lim_{\tau\to 0}\frac{1}{n!}\frac{1}{\tau}\int_V d^Nq(q^k-q_0^k)\cdots(q^l-q_0^l)G(\vec{q},\vec{q}_0,\tau) \tag{11}$$

and l is the nth index.

Owing to the δ-function nature of the short-time propagator, $G(\vec{q},\vec{q}_0,\tau)$, as $\tau\to 0$ the integration limits of the integrals over q may be taken to include all space. Hence, the first two terms cancel since the propagator is generally normalized to unity. The Gaussian character of the propagator in this limit allows the transition moments to be calculated such that[5]

$$A^{(n)}_{l,\ldots,k}=\begin{cases}K^l, & n=1\\ \frac{1}{2}Q^{lk}, & n=2\\ 0, & n\geq 3\ .\end{cases} \tag{12}$$

The term involving the transition moments becomes after partial integration

$$\int_V d^N q_0 p(\vec{q}_0,t)\left[K^i(\vec{q}_0)\frac{\partial}{\partial q_0^i}+\frac{1}{2}Q^{ij}(\vec{q}_0)\frac{\partial^2}{\partial q_0^i\partial q_0^j}\right]R(\vec{q}_0)=\int_V d^N q_0 R(\vec{q}_0)\left[-\frac{\partial}{\partial q_0^i}K^i(\vec{q}_0)+\frac{1}{2}\frac{\partial^2}{\partial q_0^i\partial q_0^j}Q^{ij}(\vec{q}_0)\right]p(\vec{q}_0,t)$$
$$+\oint dS_0 n_0^i(\vec{q}_0)\left[R(\vec{q}_0)\left[K^i(\vec{q}_0)-\frac{1}{2}\frac{\partial}{\partial q_0^j}Q^{ij}(\vec{q}_0)\right]p(\vec{q}_0,t)+\frac{1}{2}Q^{ij}(\vec{q}_0)p(\vec{q}_0,t)\frac{\partial}{\partial q_0^j}R(\vec{q}_0)\right]. \tag{13}$$

To evaluate the final term of Eq. (10) note that the following limit formula

$$\lim_{\tau\to 0}\frac{1}{\tau}\int_t^{t+\tau}F'(s)ds=\lim_{\tau\to 0}\frac{1}{\tau}[F(t+\tau)-F(t)]=F'(t)$$

enables the time integration to be performed. The previously mentioned δ-function character of the short-time propagator simply extracts the integrand from the volume integration to result in

$$-\oint dS_0 n_0^i(\vec{q}_0)\left[R(\vec{q}_0)J^i(\vec{q}_0,t)+\frac{1}{2}Q^{ij}(\vec{q}_0)p(\vec{q}_0,t)\frac{\partial}{\partial q_0^j}R(\vec{q}_0)\right] \tag{14}$$

for the final term of Eq. (10).

Owing to the arbitrariness of $R(\vec{q})$ and its gradient both in the interior and on the boundaries, the surface and volume integrands must both identically vanish. Equating the left-hand side of Eq. (10) to the sum of the right-hand side of Eqs. (13) and (14), we conclude that the Fokker-Planck equation is indeed satisfied in the interior while

$$\lim_{\tau\to 0}J^i(\vec{q}_0,t+\tau)=K^i(\vec{q}_0)p(\vec{q}_0,t)-\frac{1}{2}\frac{\partial}{\partial q_0^j}Q^{ij}(\vec{q}_0)p(\vec{q},t)$$

and

$$\lim_{\tau\to 0}p(\vec{q}_0,t+\tau)=p(\vec{q}_0,t)$$

must hold on the boundaries. We have thereby successfully reproduced both the Fokker-Planck equation and the boundary conditions from a path-integral approach. The sole requirements made on the propagator function in this section are a properly normalized δ-function nature and that it produces Gaussian character transition moments in the limit of small time intervals. Such functions satisfying the Fokker-Planck equation to order $O(\tau^2)$ are available in a wide variety of forms in the literature in addition to the simple form by Dekker mentioned above.[5,6,22–27] This proof extends and generalizes the path sum to explicitly include boundary conditions.

The construction of a continuous-time path integral from the discrete path sum is not nearly as concise for restricted stochastic processes as it is for unrestricted processes. In a numerical procedure this does not pose any significant problems to implementation since any time evolution must be based on discrete time steps (see Ref. 16 and Sec. V). However, many authors have analyzed the unrestricted path integral as a basis for a nonequilibrium thermodynamic theory.[7–10] The exponent in the propagator function can be shown to correspond to the classical Lagrangian for the most probable value of $\vec{q}(t)$. Developing the correct functional integral form from Eq. (8) for restricted processes is a significant task but may provide information into how systems interact with their external environments (through the boundary conditions).

IV. CLASSIFICATION OF BOUNDARY CONDITIONS

In dealing with the coordinate space over which Eq. (1) is valid, two generic classes of boundary conditions arise. Those which are contained implicitly in the Fokker-Planck coefficients themselves are known as singular boundaries. Such boundaries arise because of certain types of zeros or singularities in $K^i(\vec{q})$ and/or $Q^{ij}(\vec{q})$. In these cases, given regions of space may be precluded from a nontrivial solution and are inaccessible to the stochastic process. Obviously, $|\vec{q}|\to\infty$ forms such a boundary since a physically real process cannot extend beyond this limit. Singular boundaries have been further classified by the existence or nonexistence of the integrals of certain functions of K^i and Q^{ij}.[28,29] For the purposes of this paper, we note that the contribution to the surface integral in Eq. (7) by these boundaries is zero, thus the solution to Eq. (1) can be found easily if the correct Green's function is known.

The second class of boundary conditions encountered are referred to as being regular. These are externally supplied within the singular boundaries in addition to Eq. (1) and may represent a variety of physical situations. Formally, to be able to solve Eq. (7), the Green's function must be chosen in such a way to cause the unspecified terms in the surface integral to vanish. This can be accomplished by constructing a Green's function satisfying the homogeneous boundary conditions adjoint to those applied to the distribution function, $p(\vec{q},t)$.

Many physical problems can be characterized by the following two types of regular boundary conditions.[17]

(a) *Dirichlet condition.* In this case the value of the probability distribution is specified at the surface to be $p(\vec{q}_b,t)=b_D(\vec{q}_b,t)$, where b_D is a known function and $\vec{q}_b$ defines the surface. From Eq. (3), it is easily shown that the homogeneous boundary conditions adjoint to this requirement are

$$G_D(\vec{q},t;\vec{q}_0,t_0)=0 \tag{15}$$

for $\vec{q}_0$ on the surface. Then the solution to the Fokker-Planck equation with a Dirichlet-type boundary conditions becomes

$$\begin{aligned} p(\vec{q},t)=&\int_0^t dt_0 \int dv_0 \rho(\vec{q}_0,t_0) G_D(\vec{q},t;\vec{q}_0,t_0) \\ &+\int dv_0 p(\vec{q}_0,0) G_D(\vec{q},t;\vec{q}_0,0) \\ &-\tfrac{1}{2}\int_0^t dt_0 \oint dS_0 b_D(\vec{q}_0,t_0) n_0^i Q^{ij}(\vec{q}_0) \\ &\times \frac{\partial}{\partial q_0^j} G_D(\vec{q},t;\vec{q}_0,t_0) . \end{aligned} \tag{16}$$

(b) *Neumann condition.* Another frequently encountered type of boundary condition is that of a specific probability current normal to the surface, i.e.,

$$n_0^i J^i(\vec{q}_0,t)=b_N(\vec{q}_0,t) . \tag{17}$$

Again using Eq. (3), the corresponding homogeneous adjoint boundary condition is found to be

$$n_0^i \left[Q^{ij}(\vec{q}_0) \frac{\partial}{\partial q_0^j} G_N(\vec{q},t;\vec{q}_0,t_0) \right] = 0 \tag{18}$$

for $\vec{q}_b$ on the surface.

Using the function satisfying this condition, the solution to the Fokker-Planck equation with Neumann-type boundary conditions becomes

$$\begin{aligned} p(\vec{q},t)=&\int_0^t dt_0 \int dv_0 \rho(\vec{q}_0,t_0) G_N(\vec{q},t;\vec{q}_0,t_0) \\ &+\int dv_0 p(\vec{q}_0,0) G_N(\vec{q},t;\vec{q}_0,0) \\ &-\int_0^t dt_0 \oint dS_0 b_N(\vec{q}_0,t_0) G_N(\vec{q},t;\vec{q}_0,t_0) . \end{aligned} \tag{19}$$

V. BOUNDARY INTEGRAL METHOD

In actual practice, the construction of Green's functions satisfying the requirements of the preceding section may be difficult or even impossible. In particular, multidimensional problems or those involving complicated boundaries are often awkward. In these cases an integral method of evaluation Eq. (7) can be developed. Combined with the path-integral formalism, a technique to numerically solve nonlinear Fokker-Planck equations with regular boundaries is possible.

Consider as an example the slab geometry or one-dimensional problem. The path-sum solution is given by Eq. (8). From the short-time propagator, the Green's function appropriate to the two boundary conditions could be constructed. However, they generally are cumbersome series expressions.[29]

For this reason we choose to use the propagator for an unrestricted space, but subsequently must deal with some unspecified terms. Specifically, Eq. (8) becomes an integral equation of the Fredholm type in space and of the Volterra type in time.[30] In the one-dimensional problem, the surface integral collapses to the value of the integrand at the end points. In a previous paper,[16] we introduced a numerical scheme based on a histogram representation of $P(q,t)$ to solve the one-dimensional path sum in the absence of added boundary conditions. The histogram implies an averaged value of p over an interval of the q axis. However, the presence of an added regular boundary requires a good knowledge of the value of the distribution function and of the probability current at the boundary rather than for the adjacent interval in order to evaluate the surface terms of Eq. (8). For this reason we introduce as the next-higher-order approximation to $p(q,t)$ a trapezoidal representation such that

$$p(q,t)=\left[\frac{q-q_i}{q_{i+1}-q_i}\right]p_{i+1}+\left[\frac{q_{i+1}-q}{q_{i+1}-q_i}\right]p_i , \qquad q_i \le q \le q_{i+1} . \tag{20}$$

Inserting this representation into Eq. (8), integrating over q from q_i to q_{i+1}, and dividing the integral over q' into N parts yields the iterative relation

$$p_i(t+\tau)+p_{i+1}(t+\tau)=\sum_{j=1}^{N}[p_j(t)A_{ij}(\tau)+p_{j+1}(t)B_{ij}(\tau)]+S_i^P(t+\tau)+S_i^J(t+\tau) , \tag{21}$$

where

$$\begin{aligned} A_{ij}(\tau)&=\frac{2}{\Delta q_i \Delta q_j}\int_{q_i}^{q_{i+1}} dq \int_{q_j}^{q_{j+1}} dq' G(q,q',\tau)(q_{j+1}-q') , \\ B_{ij}(\tau)&=\frac{2}{\Delta q_i \Delta q_j}\int_{q_i}^{q_{i+1}} dq \int_{q_j}^{q_{j+1}} dq' G(q,q',\tau)(q'-q_j) , \end{aligned} \tag{22a}$$

and

$$S_i^P(t+\tau)=\frac{1}{\Delta q_i}\left[Q(a)\int_0^\tau d\tau' p(a,t+\tau')\int_{q_i}^{q_{i+1}} dq\frac{\partial G}{\partial a}(q,a,\tau')-Q(b)\int_0^\tau d\tau' p(b,t+\tau')\int_{q_i}^{q_{i+1}} dq\frac{\partial G}{\partial b}(q,b,\tau')\right], \tag{22b}$$

$$S_i^J(t+\tau)=\frac{2}{\Delta q_i}\left[\int_0^\tau d\tau' J(a,t+\tau')\int_{q_i}^{q_{i+1}} dq\, G(q,a,\tau')-\int_0^\tau d\tau' J(b,t+\tau')\int_{q_i}^{q_{i+1}} dq\, G(q,b,\tau')\right],$$

and

$$\Delta q_i = q_{i+1}-q_i\ .$$

In our previous paper[16] we investigated the stability of the numerical procedure with regard to the various forms of short-time propagator functions and found no significant numerical differences between them. For this reason it is sufficient to choose the simplest form of the propagator as an unrestricted Green's function. For the one-dimensional problem, the function is[24]

$$G(q,q',\tau)=\frac{1}{\sqrt{2\pi Q(q')\tau}}\exp\left[-\frac{[q-q'-K(q')\tau]^2}{2Q(q')\tau}\right]. \tag{23}$$

For this propagator function, the Fokker-Planck coefficients are to be evaluated at the source point q'. Hence the integrations over q in Eq. (22) may be evaluated in a closed form. For a general choice of K and Q, the integrations in Eq. (22a) over q' can only be performed numerically. However, once these values are calculated, they may be stored and used repeatedly since they do not change with time. The derivatives in Eq. (22b) lead to quite complicated expressions due to this dependence of the coefficients K and Q on q'. A specific simplification stems from the result that the terms involving the derivatives are of an order higher than τ^2. These terms may then be neglected as a consequence of the assumptions involved in arriving at Eq. (23). The path-integral formalism requires that the time-step approach zero for the path sum to represent the Fokker-Planck equation and the boundary conditions (Sec. III). In a numerical method, this means that τ is a small number relative to some quantity.[16] Therefore, since the probability distribution and current vary only moderately with time compared to the propagator function, we may make the substitution $p(q_b,t+\tau)\rightarrow p(q_b,t)$ or $J(q_b,t+\tau)\rightarrow J(q_b,t)$ for the unspecified terms. Equation (21) then consists wholly of known quantities and may be straightforwardly evaluated.

VI. RESULTS

In order to provide a realistic test of this numerical procedure, several example problems on the half space with exact analytic solutions representing various types of boundary conditions were investigated.

A. Homogeneous Neumann boundary condition ($J=0$)

One of the advantages of the reflecting barrier class of problems is that the probability distribution remains normalized for all time. This can be used as a feedback mechanism to reduce the error.

1. *Wiener process (constant K and Q)*

For the zero-current, one-dimensional Wiener process the exact solution is given by Eq. (B4). A negative drift force was chosen in order to drive the distribution toward the boundary and test the accuracy in that region. Figure 1 shows the probability distribution (solid line) according to the numerical evaluation of the path sum and the absolute value of the difference between the exact and this numerical solution (dashed line).

2. *Ornstein-Uhlenbeck process ($K=-\alpha x$, constant α and Q).*

For the zero-current one-dimensional Ornstein-Uhlenbeck process the exact solution is given by[29]

$$p(q,t)=\frac{1}{[2\pi v^2(t)]^{-1/2}}\left[\exp\left[-\frac{[q-m(t)]^2}{2v^2(t)}\right]+\exp\left[-\frac{[q+m(t)]^2}{2v^2(t)}\right]\right], \tag{24}$$

where

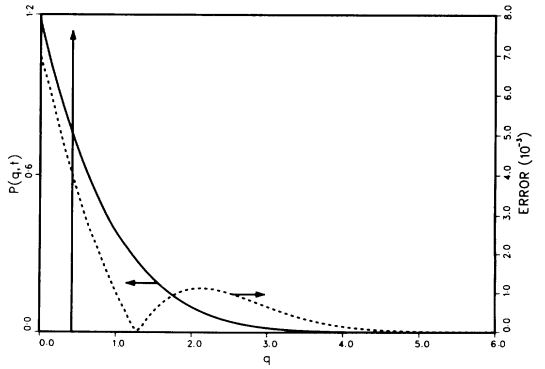

FIG. 1. Wiener process subject to the condition $KP(q,t)-\frac{1}{2}Q[\partial P(q,t)/\partial q]=0$ at $q=0$ for the time $t=1$. The solid line represents the distribution function and the dashed line represents the absolute value of the discrepancy between the numerical and analytical results. The initial condition (shown here as a vertical arrow) is a δ function centered at $q=0.42$. The time step was chosen as 0.01 with $K=1.0$ and $Q=2.0$.

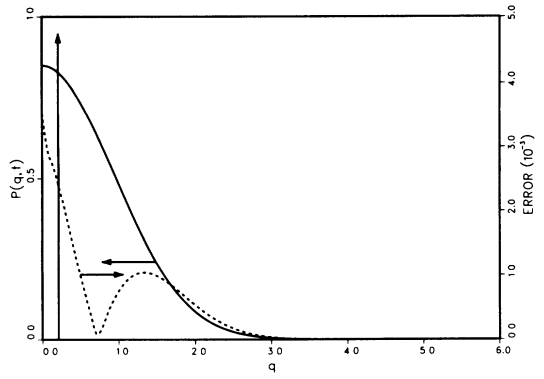

FIG. 2. Ornstein-Uhlenbeck process subject to the condition $K(q)P(q,t)-\frac{1}{2}Q[\partial P(q,t)/\partial q]=0$ at $q=0$ for the time $t=1$. The initial δ function is located at $q=0.21$. The time step is 0.0025 with $\alpha=-1.0$ and $Q=2.0$.

$$m(t)=q_0\exp(-\alpha t)$$

and

$$v^2=(Q/2\alpha)[1-\exp(-2\alpha t)] .$$

Here q_0 is the location of the initial δ function. This process presents some difficulties since $K(q)$ vanishes at $q=0$ causing the value of $S_i^P(t+\tau)$ in Eq. (22b) to apparently take on an indeterminate form. However, by application of L'Hopital's rule a definitive value can be obtained. Figure 2 shows the numerically obtained distribution function and the absolute error between the analytic and numerical results at time $t=1$.

3. *Nonlinear problems*

Unfortunately, it is difficult to analytically solve for the time dependence of nonlinear problems involving external boundary conditions. However, in many cases steady-state solutions are readily obtainable. A particular problem of interest, introduced by Clement and Wood[12] to model the size distribution of small gas bubbles is

$$K(q)=3q^{1/2}-q ,$$
$$Q(q)=3q^{1/2}+q . \tag{25}$$

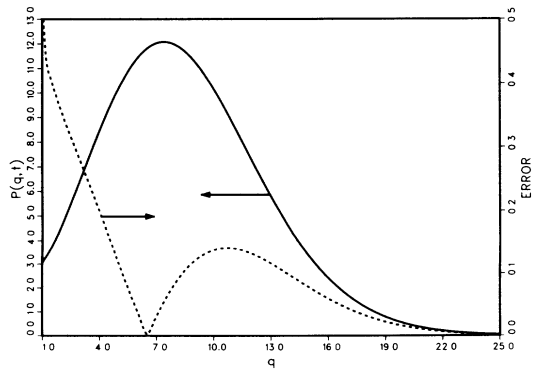

FIG. 3. Steady-state solution to the process defined by Eq. (25) subject to the condition $K(q)P(q,t)-\frac{1}{2}\{\partial[Q(q)P(q,t)]/\partial q\}=0$ at $q=1.0$. The time step was chosen as 0.01.

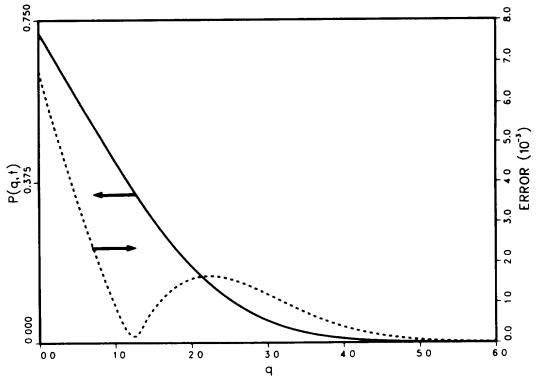

FIG. 4. Wiener process subject to the condition $KP(q,t)-\frac{1}{2}Q[\partial P(q,t)/\partial q]=J_0=1$ at $q=0$ for the time $t=1.0$. The initial distribution is zero everywhere. The time step is 0.01 with $K=1.0$ and $Q=2.0$.

A zero-current boundary condition at $q=1$ reflects the statement that the total number of particles does not change with time. The steady-state solution is given as

$$p(q)=\frac{B}{q^{1/2}}\left[1+\frac{q^{1/2}}{3}\right]^{-73} e^{(-2q+24q^{1/2})} , \tag{26}$$

where B is a constant dependent on the normalization. Figure 3 shows the steady-state results for this problem when subject to a normalization of 125.

B. Inhomogeneous Neumann boundary conditions

In Appendix B the exact solution for the one-dimensional Wiener process with a constant current maintained at $q=0$ is derived. The area under the probability distribution curve is given as the time elapsed multiplied by the current. This time dependent normalization has been included in a correction procedure discussed previously.[16] The results for this problem are given in Fig. 4.

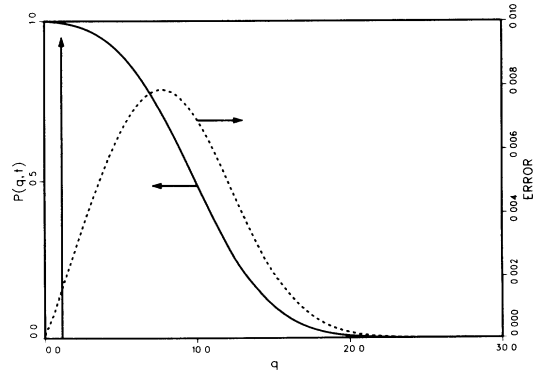

FIG. 5. Wiener process subject to the condition $P(q,t)=1.0$ and $q=0$ for the time $t=9.0$. The time step is 0.01 with $K=1.0$ and $Q=2.0$. The initial distribution is zero everywhere except at the boundary.

C. Inhomogeneous Dirichlet boundary condition

In Appendix A the exact solution for the one-dimensional Wiener process, where the value of the distribution is kept fixed at the origin, is derived. In this case the current and hence the normalization are complicated functions of the time. Figure 5 shows the results obtained for this problem.

VII. CONCLUSIONS

The effect of the boundary conditions is to add extra terms corresponding to surface source distributions to the solution of $P(\vec{q},t)$. If the Green's function appropriate to the boundary conditions is not readily available, the unrestricted Green's function may be used in Eq. (7) resulting in an integral equation to be solved. For the general nonlinear Fokker-Planck equation, the short-time propagator provides the only obtainable Green's function. The trapezoidal rule of Sec. V represents a refinement of a previously introduced numerical technique to implement path-integral concepts. Combined with the integral equation approach, a numerical technique for treating the boundary conditions of the Fokker-Planck equation is established. From Figs. 1–5, it can be seen that the numerical results are generally within a few percent of the analytic solutions.

Although no exact time-dependent solutions for nonlinear coefficients combined with external boundary conditions exist, the numerical method has previously been shown to provide correct results for unrestricted nonlinear cases also.

Accordingly, we expect our numerical method to provide accurate results for restricted nonlinear stochastic processes, as we have demonstrated in Sec. III that the path-sum solution to nonlinear Fokker-Planck equations can be extended to stochastic processes with regular boundary conditions.

APPENDIX A: EXACT SOLUTION OF THE ONE-DIMENSIONAL DIRICHLET WIENER PROCESS

Consider the one-dimensional case of constant Fokker-Planck coefficients on a half space. We seek the solution to Eq. (1) satisfying the conditions

$$\begin{aligned} &p(q,0)=0, \quad q>q_b \\ &p(q_b,t)=C, \quad t>0 . \end{aligned} \tag{A1}$$

Without loss of generality, we will take $q_b=0$. The Green's-function solution satisfying the homogeneous boundary condition can easily be found by the method of images from the well-known unrestricted solution. This so-called "absorbing" barrier solution is[29,31]

$$G_D(q,q_0,t)=\frac{1}{\sqrt{2\pi Qt}}\left(e^{-(q-q_0-Kt)^2/2Qt} - e^{-2Kq_0/Q}e^{-(q+q_0-Kt)^2/2Qt}\right) . \tag{A2}$$

Substituting Eqs. (A1) and (A2) into Eq. (8) yields

$$p(q,t)=\frac{QC}{2}\int_0^t \frac{\partial}{\partial q_0}G_D(q,q_0,t)\,|_{q_0=0}dt . \tag{A3}$$

The differentiation may be taken outside of the integral sign and with the substitution $u=t^{1/2}$, the integrals take the form

$$\int e^{-a^2u^2-b^2/u^2}du .$$

These integrals may be performed[32] with the final result

$$p(q,t)=\frac{C}{2}\left[e^{2Kq/Q}\mathrm{erfc}\left(\frac{q+Kt}{\sqrt{2Qt}}\right)+\mathrm{erfc}\left(\frac{q-Kt}{\sqrt{2Qt}}\right)\right] ,$$

where erfc is the complementary error function. This result is in agreement with previous works.[13,33,34]

APPENDIX B: EXACT SOLUTION OF THE ONE-DIMENSIONAL NEUMANN WIENER PROCESS

As a second example of a problem with an inhomogeneous regular boundary condition possessing a closed-form solution, consider the same process subject to the conditions

$$\begin{aligned} &p(q,0)=0, \quad q>q_b \\ &J(q_b,t)=Kp(q_b,t)-\frac{Q}{2}\frac{\partial}{\partial q_b}p(q_b,t)=J_0 . \end{aligned} \tag{B1}$$

Again we take $q_b=0$. The required Green's function must satisfy the homogeneous adjoint boundary condition

$$\frac{\partial}{\partial q_0}G_N(q,q_0,t)\,|_{q_0=0}=0 . \tag{B2}$$

In order to construct such a Green's function, it is necessary to express this condition in terms of the field point q. From the reciprocity relation, Eq. (4), the adjoint Neumann Green's function satisfies

$$\frac{\partial}{\partial q_0}\tilde{G}_N(q_0,q,t)\,|_{q_0=0}=0$$

or

$$\frac{\partial}{\partial q}\tilde{G}_N(q,q_0,t)\,|_{q=0}=0 .$$

From the defining relation of the adjoint boundary condition, Eq. (3), and the bilinear concomitant operator, the Neumann Green's function is found to also satisfy

$$\left[KG_N(q,q_0,t)-\frac{Q}{2}\frac{\partial}{\partial q}G_N(q,q_0,t)\right]\Bigg|_{q=0}=0 . \tag{B3}$$

This reflecting barrier solution may be constructed via an image system consisting of a point image at $q=-q_0$ and a continuous set of images in the range $-\infty<q<-q_0$,[31,35]

$$G_N(q,q_0,t)=\frac{1}{(2\pi Qt)^{1/2}}(e^{-(q-q_0-Kt)^2/2Qt}+e^{-2Kq_0/Q}e^{-(q+q_0-Kt)^2/2Qt})-\frac{K}{Q}e^{2Kq/Q}\operatorname{erfc}\left[\frac{q+q_0+Kt}{\sqrt{2Qt}}\right]. \quad \text{(B4)}$$

Inserting Eqs. (B1) and (B2) into Eq. (8) yields

$$P(q,t)=J_0\int_0^t G_N(q,q_0,t')\,|_{q_0=0}dt' . \quad \text{(B5)}$$

The first two terms in Eq. (B4) lead to integrals of the same type as involved in the previous example. The third term with the substitution $u=(t)^{1/2}$ yields integrals of the form

$$\int_0^{u_0} u\operatorname{erfc}\left[\frac{a}{u}+bu\right]du .$$

By utilizing the definition of the error function, this may be converted back to a double integral and performed by reversing the order of integrations. The result is

$$\int_0^{u_0} u\operatorname{erfc}\left[\frac{a}{u}+bu\right]du=\frac{1}{2}\left[u_0^2+\frac{a}{b}-\frac{1}{4b^2}\right]\operatorname{erfc}\left[\frac{a}{u_0}+bu_0\right]+\frac{e^{-4ab}}{8b^2}\operatorname{erfc}\left[\frac{a}{u_0}-bu_0\right]-\frac{u_0}{2b\sqrt{\pi}}e^{-(a/u_0+bu_0)^2} . \quad \text{(B6)}$$

The final solution to the Wiener process subject to an inhomogeneous Neumann boundary condition becomes

$$p(q,t)=J_0\left[\frac{1}{2K}\operatorname{erfc}\left[\frac{q-Kt}{\sqrt{2Qt}}\right]-\left[\frac{Kt}{Q}+\frac{q}{Q}+\frac{1}{2K}\right]e^{2Kq/Q}\operatorname{erfc}\left[\frac{q+Kt}{\sqrt{2Qt}}\right]+\sqrt{2t/Q\pi}e^{-(q-Kt)^2/2Qt}\right] .$$

[1] G. Nicolis and I. Prigogine, *Self-Organization in Nonequilibrium Systems* (Wiley, New York, 1977).

[2] R. Graham, *Quantum Statistics in Optics and Solid-State Physics*, Vol. 66 of *Springer Tracts in Modern Physics*, edited by G. Höhler (Springer, New York, 1973), p. 1.

[3] H. Haken, Rev. Mod. Phys. 47, 175 (1975); *Synergetics*, 2nd ed. (Springer, Berlin, 1978).

[4] A. Schenzle and H. Brand, Phys. Rev. 20, 1628 (1979).

[5] W. Horsthemke and L. Brenig, Z. Phys. B 27, 341 (1977).

[6] H. Dekker, Phys. Rev. A 19, 2102 (1979).

[7] H. Grabert and M. S. Green, Phys. Rev. A 19, 1747 (1979); H. Grabert, R. Graham, and M. S. Green, *ibid.* 21, 2136 (1980).

[8] H. Hara, Z. Phys. B 45, 159 (1981).

[9] R. Graham, in *Stochastic Nonlinear Systems*, edited by L. Arnold and R. Lefever (Springer, Berlin, 1981); in *Functional Integration, Theory and Applications*, edited by J.-P. Antoine and E. Tirapegui (Plenum, New York, 1980).

[10] H. Hasegawa, Prog. Theor. Phys. 57, 1523 (1977).

[11] F. Chen, *Introduction to Plasma Physics* (Plenum, New York, 1974); J. D. Callen *et al.*, *Plasma Physics and Controlled Nuclear Fusion Research* (IAEA, Vienna, 1975), Vol. 1, p. 645.

[12] C. F. Clement and M. H. Wood, Proc. R. Soc. London Ser. A 371, 553 (1980); M. R. Haynes and M. H. Wood, J. Nucl. Mater. 67, 155 (1977).

[13] T. T. Wang, T. K. Kwei, and H. L. Frisch, J. Polym. Sci. Part A 7, 2019 (1969).

[14] I. Goldberg, J. Aerosol Sci. 12, 11 (1981).

[15] W. G. Wolfer, C. K. Mansur, and J. A. Sprague, in *Radiation Effects in Breeder Reactor Structural Materials*, edited by M. L. Bleiberg and J. W. Bennet (American Institute of Metallurgical Engineers, New York, 1977), p. 841; N. M. Ghoniem and S. Sharafat, J. Nucl. Mater. 92, 121 (1980).

[16] M. F. Wehner and W. G. Wolfer, Phys. Rev. A 27, 2663 (1983).

[17] P. M. Morse and H. Feshbach, *Methods of Theoretical Physics* (McGraw-Hill, New York, 1953).

[18] I. Stakgold, *Green's Functions and Boundary Value Problems* (Wiley, New York, 1979).

[19] R. P. Shaw, Int. J. Heat Mass Transfer 17, 693 (1974).

[20] *New Developments in Boundary Element Methods*, Proceedings of the 2nd International Seminar, Southampton, 1980, edited by C. A. Brebbia (CML Publications, Southampton, 1980).

[21] *Boundary Element Methods*, Proceedings of the Third International Seminar, Irvine, CA, 1981, edited by C. A. Brebbia (Springer, New York, 1981).

[22] F. Langouche, D. Roekaerts, and E. Tirapegui, Nuovo Cimento B 53, 135 (1979).

[23] C. Wissel, Z. Phys. B 35, 185 (1979).

[24] H. Dekker, Physica 85A, 363 (1976).

[25] H. Haken, Z. Phys. B 24, 321 (1976).

[26] R. Graham, Z. Phys. B 26, 281 (1976).

[27] W. Horsthemke and A. Bach, Z. Phys. 22, 189 (1975).

[28] W. Feller, Ann. Math. 55, 468 (1952).

[29] N. Goel and N. Richter-Dyn, *Stochastic Models in Biology* (Academic, New York, 1974).

[30] W. Pogorzelski, *Integral Equations and Their Applications* (Pergamon, Oxford, 1966), Vol. 1.

[31] D. R. Cox and H. D. Miller, *The Theory of Stochastic Processes* (Wiley, New York, 1965).

[32] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun, Natl. Bur. Stand. Appl. Math. Ser. No. 55 (U.S., GPO, Washington, D.C., 1964).

[33] J. Crank, *The Mathematics of Diffusion* (Clarendon, Oxford, 1975).

[34] T. Oi, H. Kakihana, and T. Nomura, J. Nucl. Sci. Technol. 15, 835 (1978).

[35] A. J. Sommerfeld, *Partial Differential Equations in Physics* (Academic, New York, 1949).