A Numerical Path Sum Solution to Nonlinear Fokker-Planck Equations

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October 1981

UWFDM-432

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Abstract

Irradiation of solids by energetic particles produces a system far from its thermodynamic equilibrium. The evolution of these systems can be described by either stochastic differential equations or master equations. Often, the latter can be replaced by a so-called nonlinear Fokker-Planck equation, containing drift and diffusion functions which depend on the state variables of the system. The conditions for this replacement are briefly discussed.

Path sums and path integral solutions have recently been proposed for nonlinear Fokker-Planck equations, and their equivalence has been demonstrated. The path sums are particularly suited for numerical methods. Such a method is developed and applied to various one-dimensional Fokker-Planck equations for which analytical solutions exist. It is shown that the present numerical method gives excellent agreement with the analytical results provided the diffusion function is bounded over the entire domain of the state variables.

I. Introduction

Radiation damage to materials at elevated temperatures represents a special example of a system driven far from its thermodynamic equilibrium but attaining at the same time a quasi-stationary state. This state is characterized by an almost constant concentration of a supersaturation of vacancies and interstitials maintained in balance by the continuous generation of point defects through radiation-induced displacements and by the loss through recombination and absorption at internal sinks.

Nevertheless, from this quasi-stationary state emerges over time scales much longer than the one to reach this state new processes such as

a) the creation of a new sink structure consisting of dislocation loops, voids, and network dislocations [1];
b) the creation of a new precipitate structure in alloys either through segregation at sinks or through decomposition [2,3];
c) and in some cases and for appropriate conditions the creation of a new long-ranged order in the form of void lattices and loop lattices [4-10].

The last process in particular is a striking example of cooperative phenomena which have been termed dissipative structures by Prigogine and co-workers [10,11]. The universal significance of dissipative structures in any system driven far from equilibrium and ranging from inverted electron populations in laser systems to gene evolution in human populations has been expounded by Prigogine and co-workers (the Brussels school) and by Haken and co-workers (the Stuttgart school), and the latter have given this field of interdisciplinary research the name of Synergetics [12,13].

In order to describe mathematically such non-equilibrium systems both deterministic and stochastic aspects must be included into the evolution

equations for the parameters which characterize the dissipative or ordered structures. If we call these parameters loosely order-parameters q_α ($\alpha = 1,2...n$), then two ways have been developed to describe their evolution.

a) Langevin Method or Stochastic Differential Equations

The rate of change for the order parameters, $\dot{q}_\alpha$, is assumed to consist of a deterministic part plus a fluctuating part,

$$\dot{q}_\alpha = k_\alpha(\bar{q},t) + g_\alpha(\bar{q})L_\alpha(t) \quad . \tag{1}$$

Here, $k_\alpha(\bar{q},t)$ is a smooth function of all the order parameters and the time, whereas $L_\alpha(t)$ is a random function which is not differentiable at certain points or even anywhere. As a result, the Langevin method requires additional rules to deal with these stochastic functions $L_\alpha(t)$, such as the Ito or Stratanovich calculus. This approach is particularly suitable when the "noise" is externally generated. For fluctuations generated internally, i.e. by the system itself, the Langevin method suffers from the ambiguity that there may exist no unique prescription to separate the deterministic from the fluctuating parts. Furthermore, when the stochastic processes are restricted, i.e. when the order parameters are defined only in a finite space and need to satisfy additional boundary conditions, there does not seem to be a well defined mathematical procedure to construct the stochastic differential equations (1) such that the fluctuations $L_\alpha(t)$ do not drive the order parameters beyond the boundaries. For these reasons the following method appears to have a broader validity.

b) Master Equations

In this approach it is recognized from the very outset that the state of a system cannot be precisely ascertained because of the ever present fluctuations. Therefore, one introduces a probability distribution such that $P(\bar{q},t)dq_1 \ldots dq_n$ is the probability that the system is found to be in a state where the order parameters are between q_1 and $q_1 + dq_1$, etc. The evolution of the system is then described by transition probabilities $W(\bar{q},\bar{p})dt$ from a initial state $\bar{p}$ to a new state $\bar{q}$ within the time interval dt. As a result, the state probability function P satisfies the so-called master equation

$$\dot{P}(\bar{q},t) = \sum_{\bar{s}} W(\bar{q},\bar{q}-\bar{s})\, P(\bar{q}-\bar{s},t) - P(\bar{q},t) \sum_{\bar{s}} W(\bar{q}+\bar{s},\bar{q}) \qquad (2)$$

where the summation extends over all possible transition steps $\bar{s}$. When the order parameters are continuous variables, the sums are replaced by integrals.

The challenges one faces with the master equation approach are first the very detailed specification of the transition probability W, and second, the extraction of the deterministic and the stochastic components from the master equation.

We shall assume that the physical processes leading to transitions are clearly defined so that W can in principle be specified. When the master equation can be solved and $P(\bar{q},t)$ is known, the deterministic or average path is for example given by

$$\langle \bar{q} \rangle = \int d^n q' \bar{q}'\, P(\bar{q}',t) \quad . \qquad (3)$$

In most cases, however, the master equation is too complicated and cannot easily be solved. In these more common cases, the master equation must either be solved approximately or approximated first by a simpler evolution equation. The latter approach has proved to be the most fruitful, and it leads to a so-called Fokker-Planck equation according to the derivation presented in Section II. Although the derivation of the Fokker-Planck equation will appear straightforward, it has been and still is the subject of a lively controversy. Furthermore, the Fokker-Planck equation is not always a good approximation to the master equation over the entire space of the order parameters. Therefore, one would like to retain the master equation in that sensitive part of the parameter space, and use the Fokker-Planck equation in the remainder. However, it is presently not clear how to properly match the solutions of master and Fokker-Planck equations at their mutual boundaries.

The Fokker-Planck equation lends itself to a formal solution in terms of a path integral when the parameter domain is unrestricted. When this formal solution is expressed as a so-called path sum, however, it can be evaluated numerically. A procedure to do this is presented in Section IV, and several Fokker-Planck equations, whose analytical solutions are known, are also solved numerically. These results are presented in Section V.

Returning to the path integral formulation, it is important to note several aspects discussed in Section III. First, different path integral derivations have been given in the literature which do not always lead to the same end result. The reasons associated with these differences have, however, been illuminated more recently, and it was found that all derivations are equivalent (unless they contained an obvious mistake) as far as the path integral is concerned. However, these differences do not disappear in the path

sum formulation, and they provide additional flexibility in the choice of the numerical procedure. This flexibility will be exploited in future research to improve the accuracy of the numerical evaluation. The second point worth mentioning is that all path integral formulations presented so far are either for unrestricted processes of for those with natural boundary conditions. What is meant by the latter is that the functional form of the Fokker-Planck equation is such that it admits solutions only in a restricted domain without imposing boundary conditions. For processes restricted by extraneous or regular boundary conditions, however, a path integral formulation does not yet exist in general. For a one-dimensional process restricted to the positive axis, we present the appropriate path integral formulation in Section V. In the future, this will be generalized to multi-dimensional restricted processes.

II. The Kramers-Moyal Expansion and the Fokker-Planck Equation

Consider an arbitrary function $R(\bar{q})$ of the order parameters and multiply the master equation (2) with R. Upon integration over the entire order parameter domain we obtain

$$\int d^n R(\bar{q})\, \dot{P}(\bar{q},t) = \int d^n q \sum_{\bar{s}} W(\bar{q}+\bar{s},\bar{q})\, P(\bar{q},t)\, \{R(\bar{q}+\bar{s}) - R(\bar{q})\} \quad . \tag{4}$$

Next, we expand $R(\bar{q}+\bar{s})$ into the Taylor series

$$R(\bar{q}+\bar{s}) = \sum_{n=0}^{\infty} \frac{1}{n!} (\bar{s}\cdot\bar{\nabla})^n R(\bar{q}) \tag{5}$$

where

$$\bar{\nabla} = \left(\frac{\partial}{\partial q_1}, \frac{\partial}{\partial q_2}, \ldots\right) = (\partial_1, \partial_2, \ldots) \tag{6}$$

is the gradient operator. Then, we shift the gradient operators to act on the function

$$Q(\bar{q},\bar{s}) = W(\bar{q}+\bar{s},\bar{q})\, P(\bar{q},t) \tag{7}$$

by repeated partial integrations and obtain for the right-hand side of eq. (4) the result

$$\begin{aligned} &\int d^n q\, R(\bar{q}) \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \sum_{\bar{s}} (\bar{s}\cdot\bar{\nabla})^n Q(\bar{q},\bar{s}) \\ &+ \sum_{s} \int d\bar{\Omega}\cdot\bar{s} \sum_{n=1}^{\infty} \sum_{k=0}^{n-1} \frac{(-1)^k}{n!} [(\bar{s}\cdot\bar{\nabla})^k Q][(\bar{s}\cdot\bar{\nabla})^{n-k-1} R] \quad . \end{aligned} \tag{8}$$

The second integral is over the surface of the order parameter domain, where $d\bar{\Omega}$ is the vector normal to the surface and of magnitude equal to the local surface element.

We introduce now the notation

$$\bar{s}\cdot\bar{\nabla} = s_\alpha \partial_\alpha \quad ,$$

where summation is implied over repeated indices, and the tensor functions

$$A^{(n)}_{\alpha\beta\ldots}(\bar{q}) = \frac{1}{n!} \sum_{\bar{s}} s_\alpha s_\beta \ldots W(\bar{q}+\bar{s},\bar{q}) \tag{9}$$

where the tensor rank n is equal to the number of indices. Then the expression (8) may be written as

$$\int d^n q\, R(\bar{q}) \sum_{n=1}^{\infty} (-1)^n \partial_\alpha \partial_\beta \ldots A^{(n)}_{\alpha\beta}\ldots(\bar{q})\, P(\bar{q},t)$$

$$+ \int d\Omega_\alpha \sum_{k=0}^{\infty} \underbrace{\partial_\beta \partial_\alpha \ldots}_{k} R(\bar{q}) \sum_{n=k+1}^{\infty} (-1)^{n-k-1} \underbrace{\partial_\mu \partial_\nu \ldots}_{n-k-1} A^{(n)}_{\alpha\beta\ldots\mu\nu\ldots} P \quad .$$

Let us introduce the tensor currents

$$J^{(\ell)}_{\alpha\beta\ldots} = \sum_{n=\ell}^{\infty} (-1)^{n-\ell} \underbrace{\partial_\mu \partial_\nu \ldots}_{n-\ell} A^{(n)}_{\alpha\beta\ldots\mu\nu\ldots} P(\bar{q},t)$$

so that we can finally write for eq. (4)

$$\int d^n q\, R(\bar{q}) \left\{ \dot{P}(\bar{q},t) - \sum_{n=1}^{\infty} (-1)^n \partial_\alpha \partial_\beta \ldots A^{(n)}_{\alpha\beta\ldots} P(\bar{q},t) \right\}$$

$$= \int d\Omega_\alpha \sum_{k=0}^{\infty} J^{(k+1)}_{\alpha\beta\ldots\ldots} \underbrace{\partial_\beta \partial_\gamma \ldots}_{k} R(\bar{q}) \tag{10}$$

In order for the r.h.s of eq. (10) to vanish we must require either of two conditions:

a) Natural Boundaries

All tensor currents must vanish on the boundary $\partial\Omega$, i.e.

$$n_\alpha J^{(\ell)}_{\alpha\beta\ldots} = 0 \text{ on } \partial\Omega \text{ for } \ell = 1,2\ldots \tag{11}$$

where n_α is the normal vector on the boundary. The function $R(\bar{q})$ can be completely arbitrary both in the interior and on the boundary where it may also have arbitrary derivatives of any order.

b) Regular Boundaries

The function R is only arbitrary in the interior but not on the boundary where it is required to satisfy the conditions

$$\partial_\beta \partial_\gamma \ldots R(\bar{q}) = 0 \quad \text{on } \Omega \text{ for } k = 0,1,2,\ldots \quad . \tag{12}$$
$$k$$

For both kinds of boundaries (or a mixture thereof) the r.h.s. of eq. (10) vanishes and since $R(\bar{q})$ is an arbitrary function in the interior it follows that

$$\boxed{\frac{\partial P(\bar{q}\cdot t)}{\partial t} = \sum_{n=1}^{\infty} \frac{(-1)^n}{n!} \partial_\alpha \partial_\beta \ldots A^{(n)}_{\alpha\beta\ldots} P(\bar{q},t)} \quad . \tag{13}$$

Equation (13) is the so-called Kramers-Moyal expansion, and it is an

equivalent description of the stochastic process expressed by the master equation.

When the K-M expansion is truncated after the second term one obtains the so-called Fokker-Planck equation

$$\frac{\partial P(\bar{q},t)}{\partial t} = - \partial_\alpha [A^{(1)}_\alpha P] + \partial_\alpha \partial_\beta [A^{(2)}_{\alpha\beta} P] \quad . \tag{14}$$

If this truncation is based on the smallness of higher order moments $A^{(n)}$, a theorem by Pawula [14] asserts that if for an even n, $A^{(n)} \cong 0$, then $A^{(n)} \cong 0$ for all $n \geq 3$. If, on the other hand, the higher order even moments $A^{(n)}$ are of the same order as $A^{(2)}$, the truncation can only be made when $A^{(n)} P$ for $n > 2$ is a sufficiently smooth function so that it can be adequately approximated by a second order polynomial in the order parameters at any given point.

In the following we shall call the vector

$$A^{(1)}_\alpha = F_\alpha \tag{15}$$

the drift force and the tensor

$$A^{(2)}_{\alpha\beta} = D_{\alpha\beta} \tag{16}$$

the diffusion tensor.

Natural boundary conditions imply that

$$n_\alpha D_{\alpha\beta} P = 0 \quad \text{on} \quad \partial\Omega$$

and that the probability flux

$$n_\alpha J_\alpha = n_\alpha (F_\alpha P - \partial_\beta D_{\alpha\beta} P) = 0 \quad \text{on} \quad \partial\Omega$$

where $\partial\Omega$ is the boundary of the order parameter domain Ω and n_α its surface normal vector.

III. Path Sum and Path Integral for Unrestricted Processes

Let us consider a one-dimensional unrestricted process (or restricted process with natural boundaries) described by the Fokker-Planck equation

$$\frac{\partial P(q,t)}{\partial t} = - \frac{\partial}{\partial q} [F(q) - \frac{\partial}{\partial q} D(q)] P(q,t) \tag{17}$$

which can be interpreted as a diffusion equation with spatially dependent diffusion coefficient and drift coefficients. If F and D were constant, the solution to eq. (17) would be given by

$$P(q,t) = \int G(q,q_o,t-t_o) P(q_o,t_o) dq_o \tag{18}$$

where the Green's function or the so-called propagator is given by

$$G(q,q_o,t-t_o) = \frac{1}{\sqrt{4\pi D(t - t_o)}} \exp\{- \frac{(t - t_o)}{4D} [\frac{q - q_o}{t - t_o} - F]^2\} \quad . \tag{19}$$

If F and D depend on q, however, eq. (18) may be expected to still hold for very small time steps $\tau = t - t_o$, and for F and D taken at the prepoint q_o, i.e.

$$P(q_1,t_o+\tau) = \int G(q_1,q_o,\tau) P(q_o,t_o) dq_o \quad . \tag{20}$$

We may now iterate eq. (2) by assuming $P(q_1,t+\tau)$ is known and compute $P(q_2,t+2\tau)$, etc. The path sum is in this manner obtained and given by

$$P(q_n,t_o+n\tau) = \int \frac{dq_{n-1}}{\sqrt{4\pi D(q_{n-1})}} \cdots \int \frac{dq_o}{\sqrt{4\pi D(q_o)}} \exp\{- \sum_{i=0}^{n-1} \Delta L_i \tau\} P(q_o t_o) \tag{21}$$

where

$$\Delta L_i = \frac{1}{4D(q_i)} \left[\frac{q_{i+1}-q_i}{\tau} - F(q_i)\right]^2 . \tag{22}$$

If we now go to the limit $n \to \infty$, $\tau \to 0$ such that $n\tau$ remains finite, the path integral is obtained, and it can be written in the symbolic manner

$$P(q,t) = \int D\left(\frac{q(t)}{4\pi D(q)}\right) \exp\left\{-\int_{t_o}^{t} L(\dot{q},q)dt'\right\} P(q_o t_o) \tag{23}$$

where $q(t')$ is any path starting at $q(t_o) = q_o$ and ending at $q(t) = q$, and the integration symbol $D(\ )$ indicates a summation of <u>all</u> such possible paths. The Lagrange functional is given by

$$L(\dot{q},q) = \frac{1}{4D(q)} [\dot{q} - F(q)]^2 \tag{24}$$

and its integral $\int_{t_o}^{t} Ldt'$ is referred to as the Onsager-Machlup functional.

The above formulation of the path integral is due to Dekker [15].

Unfortunately, other path-integral formulations have appeared in the literature which do not agree with the one outlined above [16-21]. The reasons for the differences (if not simply due to errors) are associated with two issues:

a) In the discrete (or time) lattice representation of the path integral, eq. (21), the drift and diffusion coefficients need not necessarily be taken at the prepoint q_i. In fact, they can be taken also at the postpoint

q_{i+1}, at a point in between, or a combination of values at the prepoint and the postpoint may be taken. This will in general result in a different Lagrangian and a different integral measure D( ).

b) A particular Lagrangian with its appropriate measure D( ) demands a specific discrete representation of the path integral by a path sum of the form of eq. (21). What particular form one likes to choose depends on how one wants to evaluate the path integral or path sum.

Unfortunately, little can be said in quantitative terms at the present time as to what form of the Lagrangian is best suited for numerical or analytical evaluation.

Without further discussing the various path integral representation, we give a list of some of the Lagrangians proposed in the literature together with their path sum counterparts and measures in Table 1. As shown in ref. [26], all these are equivalent representations in the sense that the path integrals give identical results. However, the different path sums are expected to yield somewhat different results. This is analogous to the different numerical procedures to evaluate Riemannian integrals by discrete sums. Different numerical procedures result in identical answers only in the limit of infinitesimally small intervals. Similarly, different path sums converge to the same path integral in the limit of an infinitely large number of iterations.

Table 1. Path Integrals and Path Sums for the One-Dimensional, Nonlinear Fokker-Planck Equation

Lagrangian	Exponent in Propagator	Measure
$\frac{1}{4D}(\dot{q} - F)^2$	$\frac{\tau}{4D_i}\left[\frac{\Delta q_i}{\tau} - F_i\right]^2$ where: $\Delta q_i = q_{i+1} - q_i$ $D_i = D(q_i)$, $F_i = F(q_i)$	$\frac{dq_i}{\sqrt{4\pi\tau D_i}}$
$\frac{1}{4D}[\dot{q} - F + 2\alpha D']^2 - \alpha[F' - \alpha D'']$ where: $D' = dD/dq$ and $0 \leq \alpha \leq 1$	$\frac{\tau}{4D(\bar{q}_i)}\left[\frac{\Delta q_i}{\tau} - F(\bar{q}_i) + 2\alpha D'(\bar{q}_i)\right]^2$ $- \alpha\tau[F'(\bar{q}_i) - \alpha D''(\bar{q}_i)]$ where: $\bar{q}_i = q_i + \alpha\Delta q_i$	$\frac{dq_i}{\sqrt{4\pi\tau D(\bar{q}_i)}}$
$\frac{1}{4D}[\dot{q} - F + 2\alpha D']^2 - \alpha[F' - (2\alpha - 1)D'']$ where: $0 \leq \alpha \leq 1$	$\frac{\tau}{4\bar{D}_i}\left[\frac{\Delta q_i}{\tau} - \bar{B}_i\right]^2 - \tau\bar{C}_i$ where: $\bar{D}_i = (1 - \alpha)\, D_i + \alpha D_{i+1}$ $\bar{B}_i = (1 - \alpha)[F_i - 2\alpha D_i'] + \alpha[F_{i+1} - 2\alpha D_{i+1}']$ $\bar{C}_i = -\alpha F_i' + \alpha(2\alpha - 1)D_i''$	$\frac{dq_i}{\sqrt{4\pi\tau\bar{D}_i}}$

Table 1. (Continued)

Lagrangian	Exponent in Propagator	Measure
$\frac{1}{4D}\left[\dot{q} - F + \frac{1}{2}D'\right]^2$ $+ \alpha\sqrt{D}\,\frac{d}{dq}\,\frac{1}{\sqrt{D}}\left[F - \frac{1}{2}D'\right]$ where: $0 \leq \alpha \leq 1$	$\frac{\tau}{4\tilde{D}_i}\left[\frac{\Delta q_i}{\tau} + \tilde{B}_i\right]^2 - \tau\tilde{C}_i$ where: $\tilde{D}_i = \sqrt{D_{i+1}}\left[2\sqrt{D_{oi}} - \frac{1}{2}\sqrt{D_{i+1}} - \frac{1}{2}\sqrt{D_i}\right]$ $D_{oi} = D\left(\frac{1}{2}q_{i+1} + \frac{1}{2}q_i\right)$ $\tilde{B}_i = \sqrt{D_{i+1}}\left[(1-\alpha)\,b_i + \alpha b_{i+1}\right]$ $b_i = -F_i/\sqrt{D_i} + \frac{1}{2}D_i'$ $\tilde{C}_i = \alpha\sqrt{D_i}\,db_i/dq_i$	$\frac{dq_i}{\sqrt{4\pi\tilde{D}_i}}\sqrt{\frac{D_i}{D_{i+1}}}$
$\frac{1}{4D}\left[\dot{q} - F + \frac{1}{2}D'\right]^2$ $+ \alpha\sqrt{D}\,\frac{d}{dq}\,\frac{1}{\sqrt{D}}\left[F - \frac{1}{2}D'\right]$ $+ \frac{1}{2}\dot{q}\,\frac{D'}{D}$	same as above but with the additional term $\frac{1}{2}\Delta q_i D_{oi}'$	$\frac{dq_i}{\sqrt{4\pi\tilde{D}_i}}$

IV. Numerical Procedure to Solve the Path Sum

A numerical procedure to solve the Fokker-Planck eq. (17) is to carry out repeated iterations of eq. (20) by solving the integral numerically. To accomplish this in the most economic fashion, the integral in eq. (20) should be replaced by a sum containing a propagator matrix whose elements are determined only once and which can be used in every iteration. To find this propagator matrix, we assume first that the probability density can be represented with sufficient accuracy by a histogram as given by

$$P(q,t) = \sum_{i=1}^{N} \pi(q - q_i)\, P_i(t) \quad , \tag{25}$$

and as shown schematically in Fig. 1. Here

$$\pi(q - q_i) = \begin{cases} 1 & \text{for } q_i - \frac{1}{2}\,\Delta q_{i-1} \leq q \leq q_i + \frac{1}{2}\,\Delta q_i \\ 0 & \text{otherwise} \quad . \end{cases} \tag{26}$$

The grid points need not be equally spaced, i.e. the intervals Δq_i need not be equal. In fact, as we shall show shortly, when the diffusion function $D(q)$ is not constant, a variable grid spacing is required.

After substitution of the histogram representation into eq. (20) we integrate over the interval centered at the grid point q_i and obtain

$$P_i(t+\tau)\,\frac{1}{2}\,(\Delta q_{i-1} + \Delta q_i) = \sum_{j=1}^{N} P_j(t) \int_{(q_i - \frac{1}{2}\Delta q_{i-1})}^{(q_i + \frac{1}{2}\Delta q_i)} dq \int_{(q_j - \frac{1}{2}\Delta q_{j-1})}^{(q_j + \frac{1}{2}\Delta q_j)} dq'\; G(q,q',\tau) \quad .$$

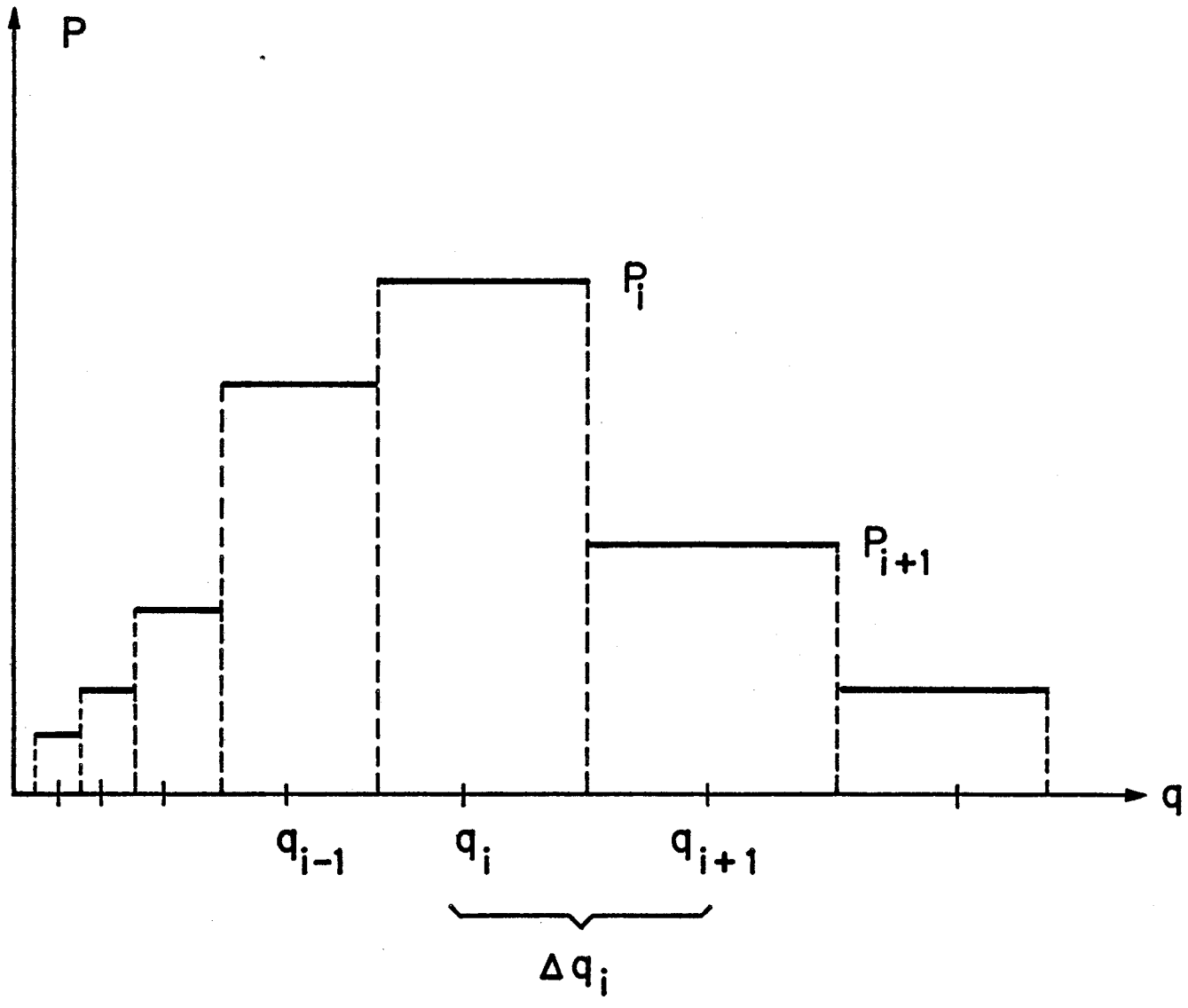

Fig. 1. Histogram representation of the distribution function.

We may now define the propagator matrix as

$$T_{ij}(\tau) = \frac{2}{\Delta q_{i-1} + \Delta q_i} \int_{(q_i - \frac{1}{2}\Delta q_{i-1})}^{(q_i + \frac{1}{2}\Delta q_i)} dq \int_{(q_j - \frac{1}{2}\Delta q_{j-1})}^{(q_j + \frac{1}{2}\Delta q_j)} dq'\, G(q,q',\tau) \tag{27}$$

so that

$$P_i(t + \tau) = \sum_{j=1}^{N} T_{ij}(\tau)\, P_j(t) \quad . \tag{28}$$

Note that for a given time step the propagator matrix needs to be evaluated only once, and it can then be used repeatedly to compute the time evolution of the histogram with eq. (28).

For the present selection of the path sum, F and D depend on the prepoint q'. As a result we can carry out the integration over the postpoint q in closed form, and we obtain

$$T_{ij}(\tau) = \frac{1}{(\Delta q_{i-1} + \Delta q_i)} \int_{(q_j - \frac{1}{2}\Delta q_{j-1})}^{(q_j + \frac{1}{2}\Delta q_j)} dq' \left\{ \operatorname{erf}\left[\frac{q_i + \frac{1}{2}\Delta q_i - q' - \tau F(q')}{\sqrt{4\pi D(q')}}\right] \right. \tag{29}$$

$$\left. - \operatorname{erf}\left[\frac{q_i - \frac{1}{2}\Delta q_{i-1} - q' - \tau F(q')}{\sqrt{4\tau D(q')}}\right] \right\} \quad .$$

The remaining integration over the prepoint interval is carried out numerical-

ly. The resulting propagator matrix is banded, with the dominant elements along the diagonal and off-diagonal elements decreasing rapidly with increasing distance from the diagonal. In the limit of $\tau \to 0$, the propagator matrix degenerates into the unity matrix δ_{ij}. The width of the band of significant elements in T_{ij} increases with τ. The banded structure of T_{ij} implies that much fewer than N^2 elements need to be computed and stored, and that the matrix operations involved in eq. (28) require much less computations.

Since eq. (28) is an approximation to the path sum of eq. (20), some numerical error is incurred in each iteration. If this error is biased, as one must expect, repeated iterations with eq. (28) will lead to a rapid accumulation of errors, and the discrete probability distribution P_i will either decrease or increase exponentially with time.

A simple correction procedure can be employed to avoid this numerical instability in case the probability distribution is normalizable. After each iteration, the sum

$$\sum_{i=1}^{N} P_i(t)\ \Delta q_i = 1 + \varepsilon \tag{30}$$

is determined. The exact probability distribution, when integrated over the order parameter q, will of course result in a value of unity without an error ε. Therefore, the discrete probability distribution is first renormalized to

$$P_i(t) \to \frac{1}{1+\varepsilon} P_i(t)$$

before being used on the r.h.s. of eq. (28) for a new iteration. It was found

in all cases considered and tested that this renormalization is essential, indicating that the error is always biased.

In restricted stochastic processes, probability may not always be conserved. For such cases other renormalization or correction procedures must be developed.

The choice of the time step τ and the interval spacing and sizes Δq_i are intimately related. This can easily be seen by considering only a diffusion process without drift. According to the Einstein relation

$$D(q) = \frac{1}{2} (\Delta q)^2/\tau \quad , \tag{31}$$

where $(\Delta q)^2$ is the mean square displacement during a time interval of τ.

We may view the histogram $P_i(t)$ as an approximation for a discrete superposition of Gaussian distributions centered around the grid points. During the time τ, these distributions broaden, and, when a drift exists, they also shift. To determine τ, we now require that the drift of the mean of one of these Gaussians will be less than the width, or the interval size Δq.

Since the drift is given by $F(q)\tau$, this requirement implies that

$$\Delta q \leq F(q)\tau \quad .$$

Using the Einstein relation (31), we find

$$\tau \leq \frac{2D(q)}{[F(q)]^2} \quad . \tag{32}$$

The condition (32) is used to select a time step τ. We require it to be ful-

filled over the region of q where the distribution function P(q,t) has an appreciable value. Once τ is selected, eq. (31) is used to find a compatible interval spacing according to

$$\Delta q_i = \sqrt{2\tau D(q_i)} \tag{33}$$

where the grid points q_i are in the center of the interval Δq_i.

V. Results

In order to test the usefulness, accuracy, and limitations of the numerical path sum methods, various Fokker-Planck equations were solved by this method and compared to the exact analytical solutions known for these cases.

a) The Wiener Process

Wiener processes are characterized by a Fokker-Planck equation with a constant drift and diffusion coefficient. If the initial distribution is given by

$$P(q,o) = \delta(q - q_o) \quad , \tag{34}$$

then the probability distribution at $t > 0$ is

$$P(q,t) = [4\pi Dt]^{-1/2} \exp\{- \frac{(q - q_o - Ft)^2}{4Dt}\} \quad . \tag{35}$$

Since both F and D are constant, an equal interval spacing can be chosen in this case except for the two intervals at either end which extend to infinity. However, the end intervals are chosen such that the value of the probability function is negligibly small.

The initial delta function was approximated by a rectangular distribution within one interval, centered at the position indicated by the vertical arrow in Fig. 2. The spreading and shift of the initial delta-distribution is shown in Fig. 2 after 80 iterations. The histogram distribution is in excellent agreement with the exact distribution.

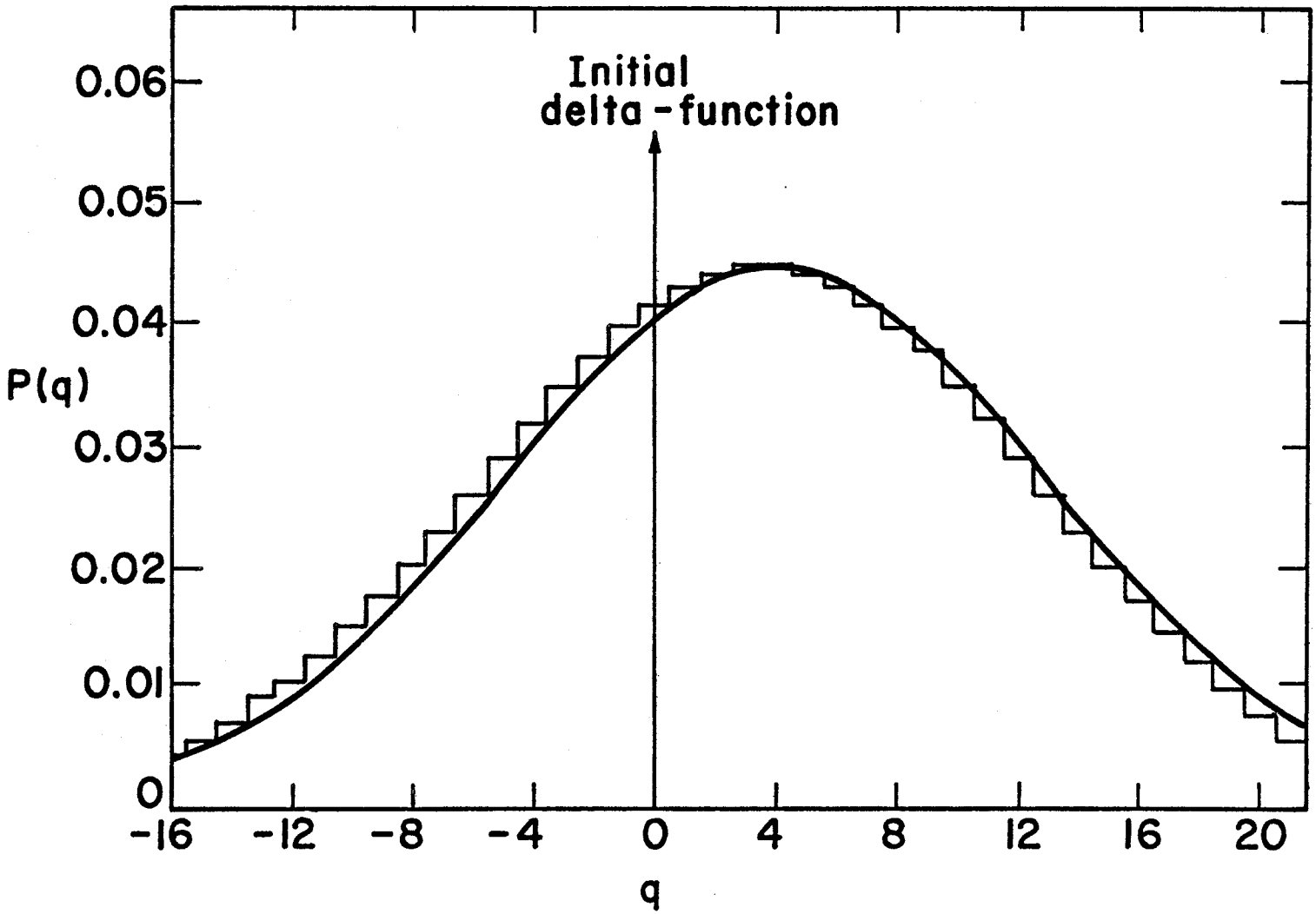

Fig. 2. Wiener process with F = D = 1, τ = 0.5, Δq = 1, after 80 iterations.

b) The Ornstein-Uhlenbeck Process

For this stochastic process, the diffusion function is a constant, whereas the drift is a linear function, i.e.

$$F = -\alpha q \quad . \tag{36}$$

The exact distribution for an initial delta-distribution is given by [27]

$$P(q,t) = [2\pi V^2(t)]^{-1/2} \exp\{-\frac{[q - m(t)]^2}{2V^2(t)}\} \tag{37}$$

where the mean is changing with time according to

$$m(t) = x_0 \exp(\alpha t) \tag{38}$$

and the covariance according to

$$V^2(t) = (\frac{D}{\alpha})[1 - \exp(-2\alpha t)] \quad . \tag{39}$$

If we want to use eq. (32) to determine the maximum allowable time step τ we need to define first those values of q_{max} for which the distribution function becomes negligible. Since the drift is negative for positive α, the distribution will tend to shift towards the origin. Thus, we may assume that $q_{max} \cong 2q_0$, where q_0 is the center of the initial δ-distribution. Hence

$$\tau \leq \frac{2D}{4\alpha^2 q_0^2} \quad .$$

Since D is constant, the intervals can again be made equidistant and selected in accordance with eq. (33).

The relaxation of a delta-function located initially at $q_0 = 10$ according to the Ornstein-Uhlenbeck process is shown in Fig. 3. Again, excellent agreement is obtained between the exact and the path sum method.

c) A Restricted Ornstein-Uhlenbeck Process

In order to test the path sum approach for a restricted process, an Ornstein-Uhlenbeck process is considered for the positive domain $0 \leq q < \infty$ only. The distribution function must therefore satisfy the boundary condition

$$\frac{dP(0,t)}{dq} = 0 \quad . \tag{40}$$

This can be accomplished by selecting the new propagator [28]

$$\begin{aligned} G(q,q_0,\tau) = [4\pi\tau D(q_0)]^{-1/2} * \{ & \exp[-\frac{(q - q_0 - \tau F(q_0))^2}{4\tau D(q_0)}] \\ & + \exp[\frac{qF(q_0)}{D(q_0)}] \exp[-\frac{(q + q_0 + \tau F(q_0))^2}{4\tau D(q_0)}] \\ & + [\frac{F(q_0)}{D(q_0)}] \exp[-\frac{qF(q_0)}{D(q_0)}] \operatorname{erfc}[\frac{q + q_0 + \tau F(q_0)}{\sqrt{2\tau D(q_0)}}]\} \end{aligned} \tag{41}$$

which is then integrated over both q and q_0 within the intervals Δq_i and Δq_j, respectively. The resulting expression for the propagator matrix $T_{ij}(\tau)$ is too lengthy and will be omitted here.

The closed form solution to this restricted Ornstein-Uhlenbeck process is given by [27]

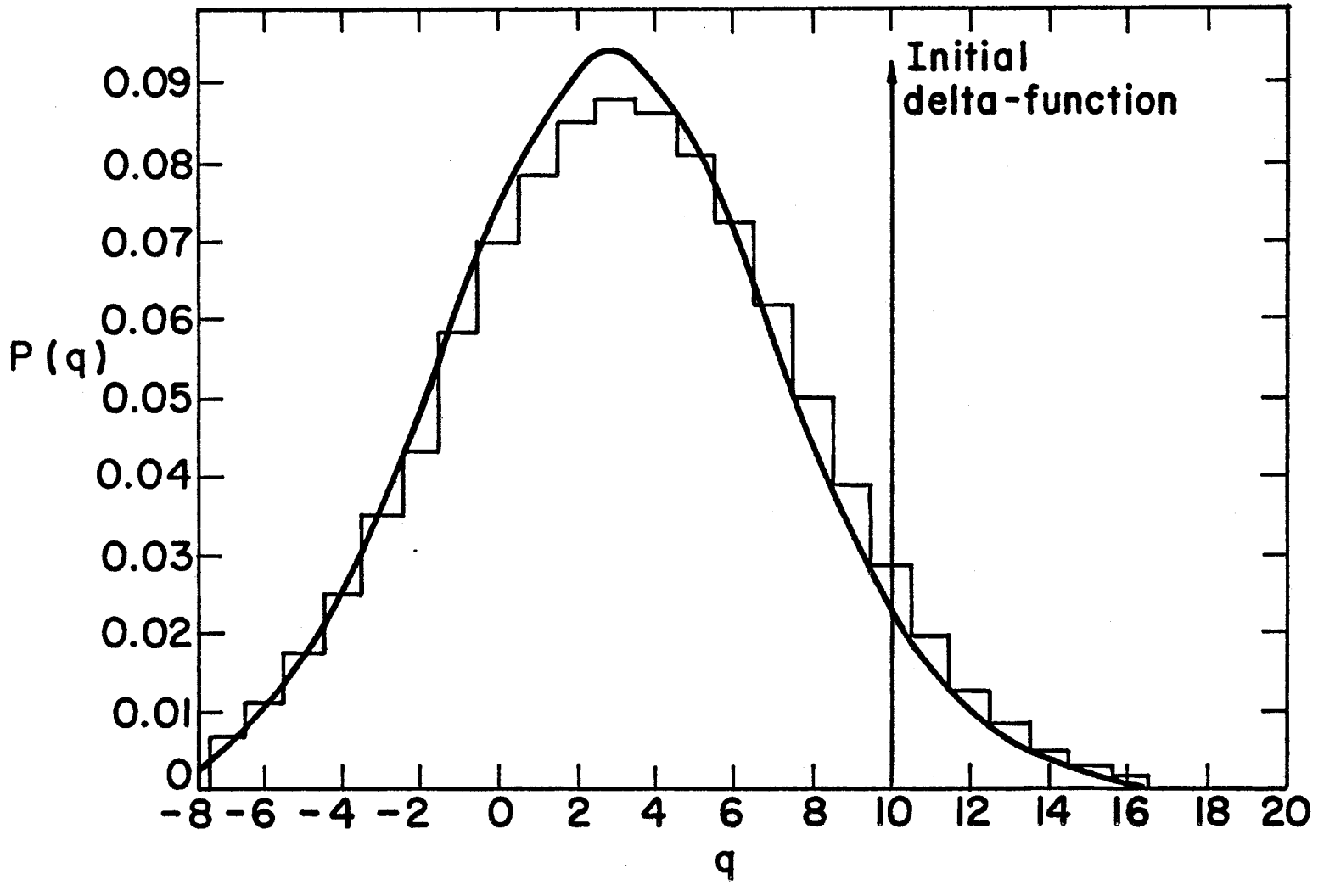

Fig. 3. Ornstein-Uhlenbeck Process with α = -0.05, Δq = 1, and τ = 0.5. Relaxation of a Delta function at q_0 = 10 after 50 iterations.

$$P(q,t) = [8\pi V^2(t)]^{-1/2}\{\exp[-\frac{(x - m(t))^2}{2V^2}] + \exp[-\frac{(x + m(t))^2}{2V^2}]\} \qquad (42)$$

when the initial distribution is a delta-function. Figure 4 shows the comparison between the exact result (solid smooth curve) and the numerical path sum result. Again, the overall agreement is excellent.

d) The Rayleigh Gas

The Rayleigh gas is a model system consisting of a dilute concentration of heavy atoms in a gas of light atoms [29]. Assuming hard sphere collisions, the Boltzmann collision equation can be reduced to a Fokker-Planck equation for the energy spectrum of the heavy particles. This equation has a drift function of

$$F = -q + \frac{3}{2} \qquad (43)$$

and a diffusion function of

$$D = q \quad . \qquad (44)$$

Since the particle energy can only be positive, this Fokker-Planck equation describes a restricted process, $0 \leq q < \infty$, with an inaccessible natural boundary at $q = 0$.

When the initial energy distribution of the heavy particles is a delta-function $\delta(q - q_0)$, then the distribution function is given by [29]

$$P(q,t) = \frac{1}{2}\exp(\frac{t}{2})[\pi q_0 \sigma]^{-1/2} * \{\exp[-\sigma^{-1}(q^{1/2} - p^{1/2})^2] - \exp[-\sigma^{-1}(q^{1/2} + p^{1/2})^2]\} \qquad (45)$$

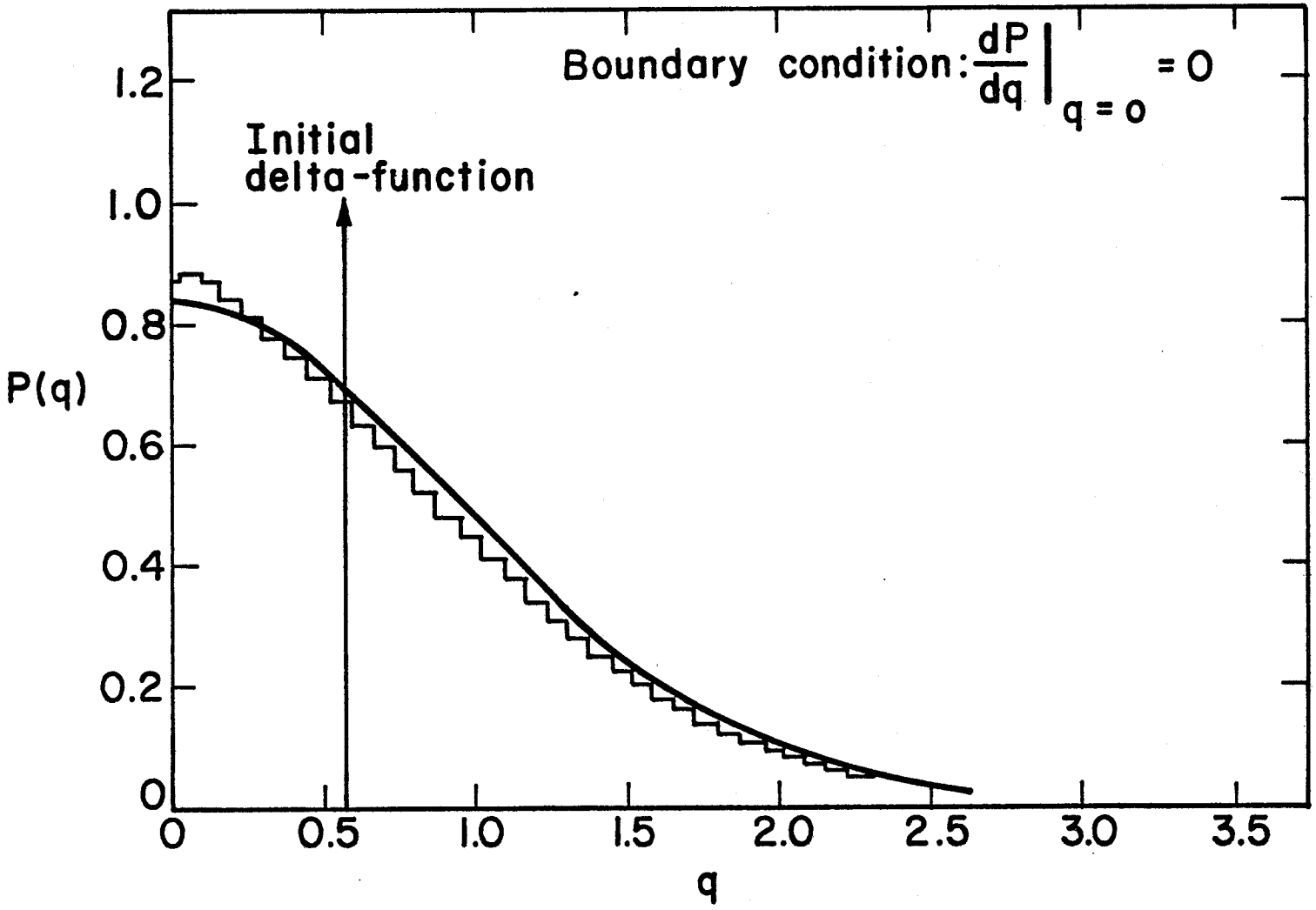

Fig. 4. Restricted Ornstein-Uhlenbeck process with $\alpha = -1$, $D = 1$, $\tau = 0.0025$ after 400 iterations.

where

$$\sigma = 1 - \exp(-t) \tag{46}$$

$$p = q_0 \exp(-t) \quad . \tag{47}$$

When the initial distribution is a Maxwellian, i.e.

$$P(q,0) = 2\left(\frac{q}{\pi}\right)^{1/2} \alpha_0^{-3/2} \exp\left(-\frac{q}{\alpha_0}\right) \quad , \tag{48}$$

the relaxed distribution is given by [29]

$$P(q,t) = 2\left(\frac{q}{\pi}\right)^{1/2} \alpha^{-3/2} \exp\left(-\frac{q}{\alpha}\right) \quad . \tag{49}$$

Here, α_0 is a parameter characterizing the temperature of the initial distribution, and

$$\alpha(t) = 1 + (\alpha_0 - 1) \exp(-t) \quad . \tag{50}$$

When we apply the criterion for choosing the time step τ, we find that

$$\tau \leq \frac{2D(q)}{F^2(q)} = \frac{2q}{(q - \frac{3}{2})^2} \tag{51}$$

which cannot be satisfied with a non-zero value of τ over the entire domain $0 < q < \infty$. For $\tau = 0.01$, the numerical procedure can be expected to be accurate only in the range $0.011 < q < 203$, and for $\tau = 0.0025$ in the range $0.0028 < q < 803$.

Figure 5 gives an example for the relaxation of a delta-function. For the partial relaxation after a time of $t = 0.3$, the distribution function has

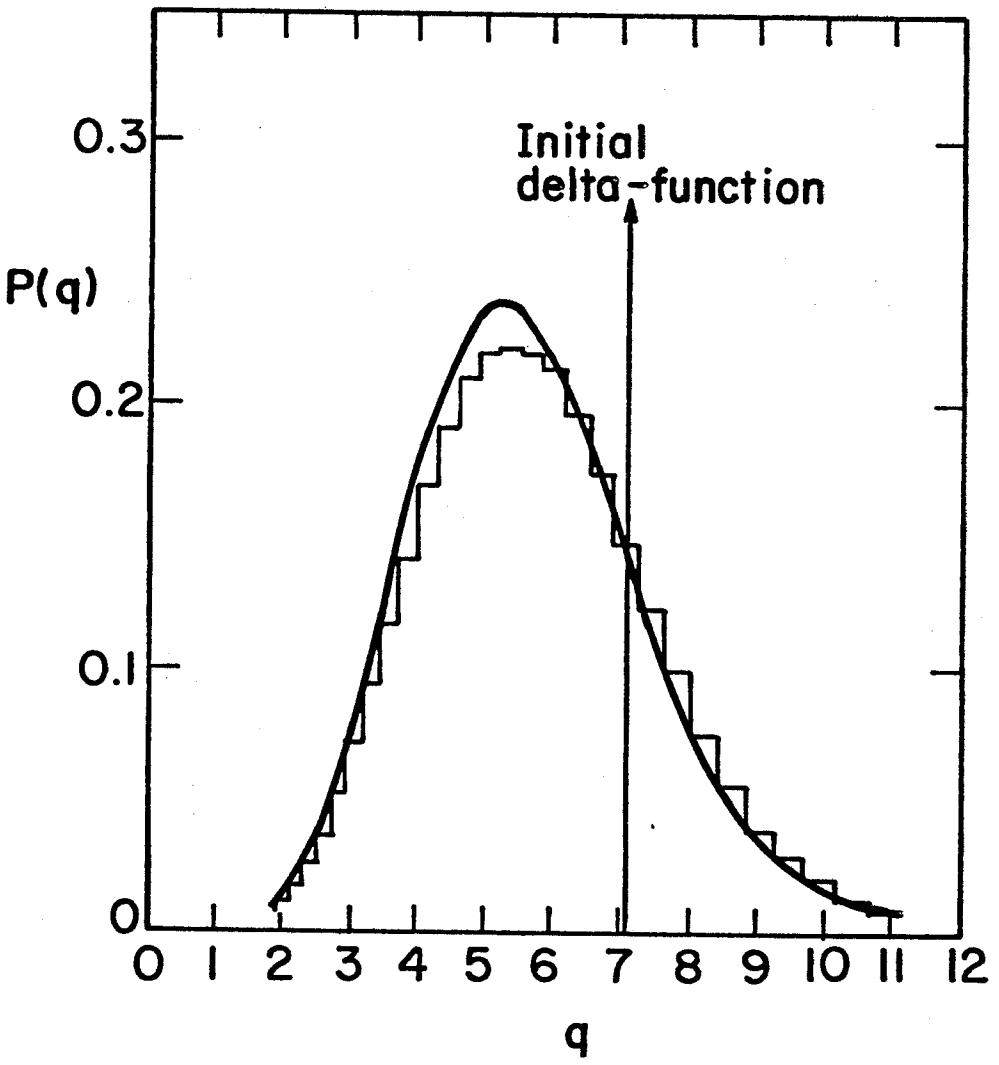

Fig. 5. Rayleigh gas relaxation from an initial delta-function distribution. The time step is $\tau = 0.01$ and the time elapsed to the relaxed distribution is $t = 0.3$.

negligible value below $q \simeq 1.5$. As a result, the numerical path sum method agrees closely with the analytical solution of eq. (45).

When the relaxation of an initial Maxwellian distribution is considered, however, a close agreement can no longer be achieved, because the distribution function has large finite values for very small values of q where our numerical path sum method breaks down.

Figures 6 and 7 illustrate the degree of discrepancy obtained. Curve b in Fig. 7 represents the initial distribution. After a short time of $t = 0.25$ has elapsed, the agreement between the exact result of eq. (49) (curve a) and the numerical result (curve c) is still satisfactory. However, for $t = 1.0$, the disagreement has become substantial as shown in Fig. 7.

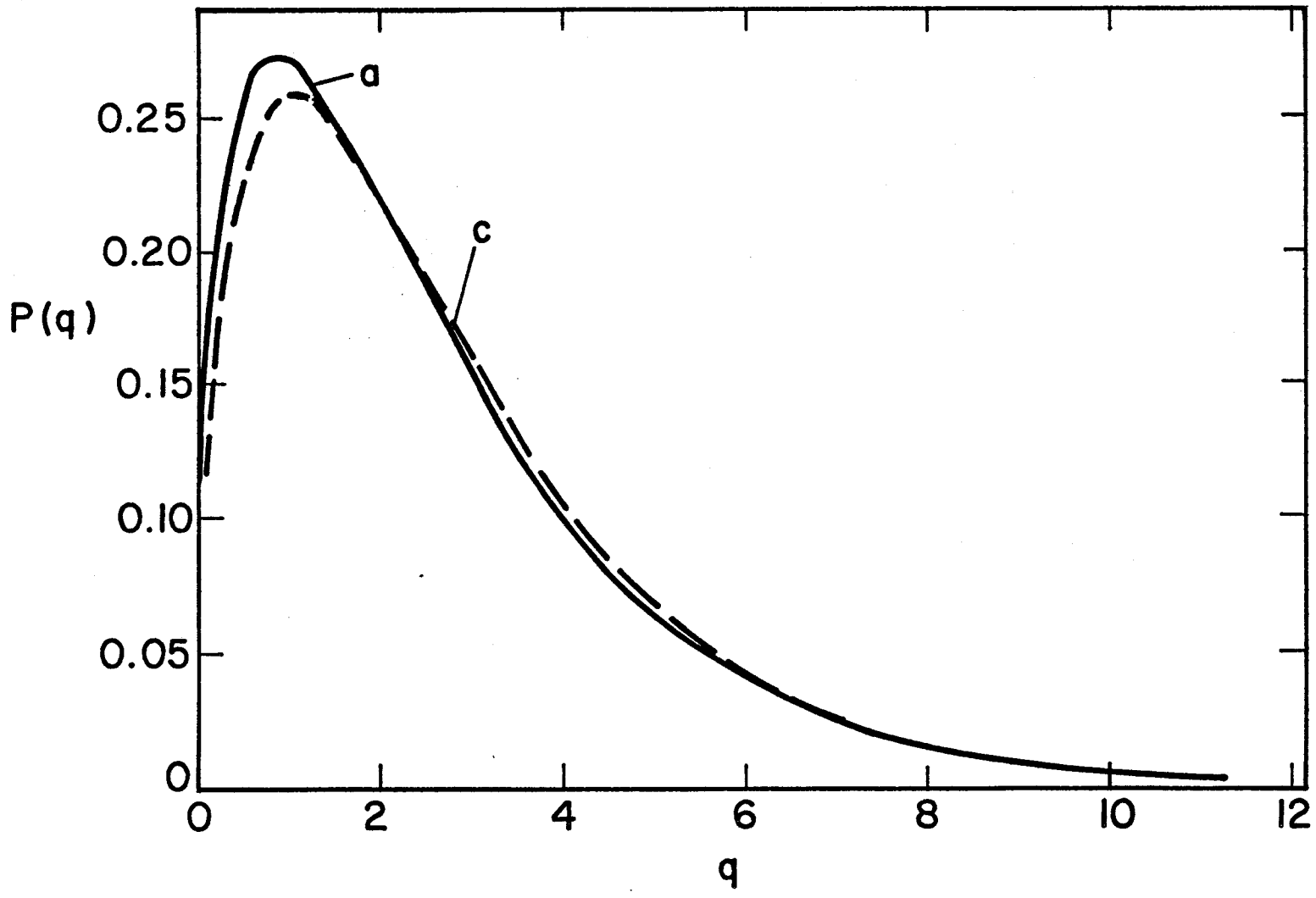

Fig. 6. Rayleigh gas relaxation from an initial distribution with $\alpha_0 = 2$ after 100 time steps of $\tau = 0.0025$. Curve a: exact result; curve c: numerical result.

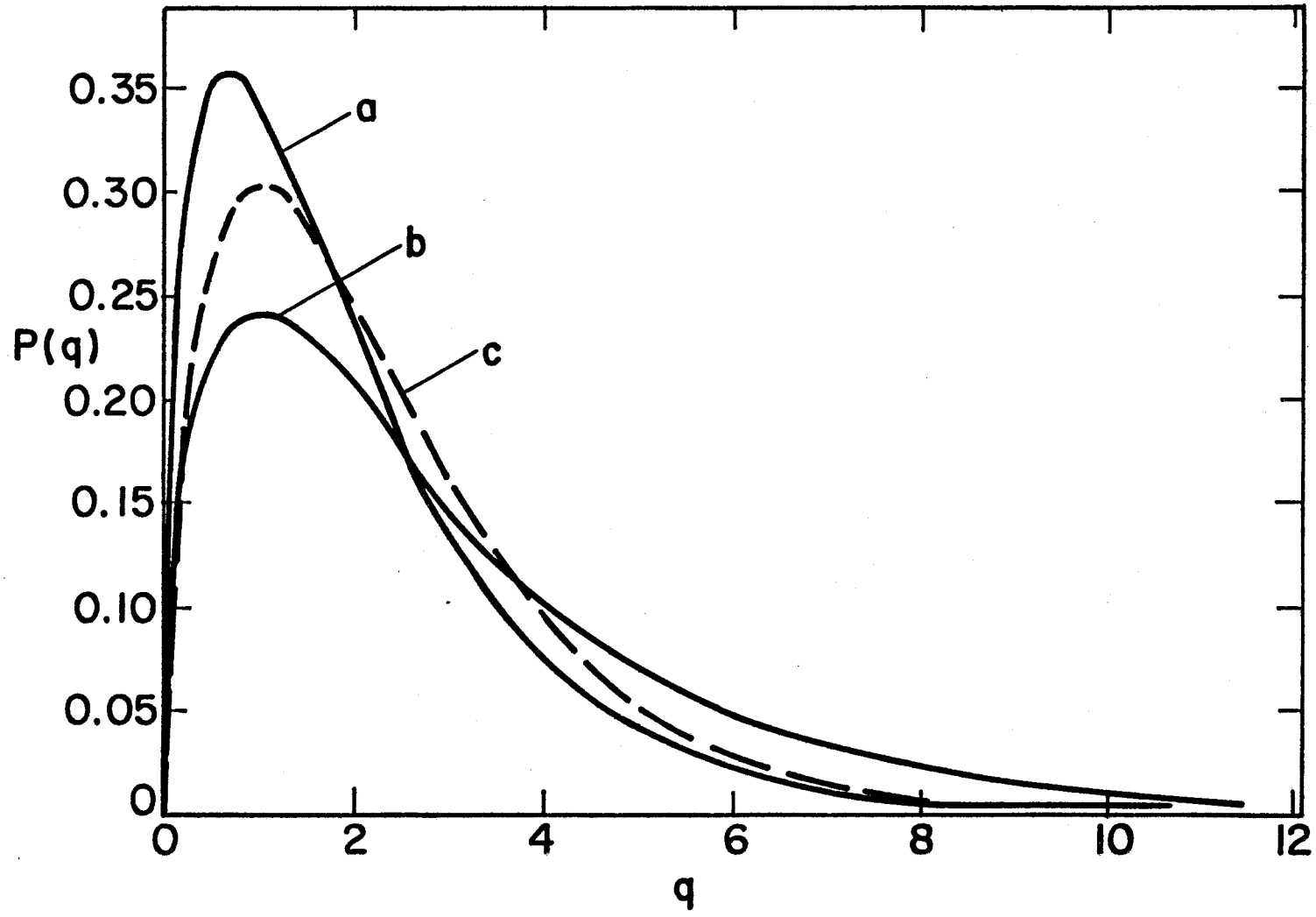

Fig. 7. Rayleigh gas relaxation from an initial distribution with $\alpha_0 = 2$ (curve c) after 400 time steps of $\tau = 0.0025$. Curve a: exact result; curve b: numerical result.

VI. Conclusions

The evolution of systems far from a thermodynamic equilibrium is best formulated in terms of a master equation. This equation can often be replaced by the simpler Fokker-Planck equation with a drift and a diffusion function depending on the parameters of the system. The Fokker-Planck equation can be solved by a path sum for which different formulations have been presented in the recent literature.

A procedure is developed for a one-dimensional Fokker-Planck equation which provides a highly efficient way for numerical solution. This numerical method is compared with existing analytical solutions of certain Fokker-Planck equations. Excellent agreement is obtained provided the diffusion function of the Fokker-Planck equation remains finite over the entire parameter space.

Acknowledgment

Support for this work has been provided by the U.S. Department of Energy, Basic Energy Science Division under contract ER-78-S-02-4861 with the University of Wisconsin.

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