JOURNAL OF COMPUTATIONAL PHYSICS 23, 425–445 (1977)

Numerical Solution of the Fokker–Planck Equation via Chebyschev Polynomial Approximations with Reference to First Passage Time Probability Density Functions

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Received March 1, 1976; revised September 21, 1976

Chebyschev approximations are employed to solve the one-dimensional, time-dependent Fokker–Planck (forward Kolmogrov) equation in the presence of two barriers a finite "distance" apart. Solutions are presented for the fundamental intervals $(-1, +1)$ and $(0, +1)$. In order to speed up the calculations, sparse matrix routines are utilized. The first passage time probability density function is also evaluated. Illustrative numerical results are presented for the Wiener process with drift, and the Ornstein–Uhlenbeck process for a variety of combinations of boundary conditions.

1. INTRODUCTION

The Fokker–Planck (forward Kolmogorov) equation arises in a wide variety of problems of physical and biological interest. Many of these problems involve the Fokker–Planck equation in the presence of two barriers (boundaries) on a finite section of the line rather than on the infinite line for which methods have been devised (see [1, 2, 15]).

When the boundaries are located a finite "distance" apart, then we have to contend with two radically different situations. In the first situation (and the one we cover in the present paper), the infinitesimal transition moments do not vanish identically at *both* boundaries. This is termed the *regular* case and essentially amounts to solving the Fokker–Planck equation subject to boundary conditions at the barriers which are generally absorbing or reflecting. When both infinitesimal transition moments vanish identically at both boundaries, this is termed the *singular* case and has been thoroughly analyzed by Feller [4]. Convenient pedagogic versions are available in Kielson [7] and Goel and Richter-Dyn [6]. The singular case is constantly encountered in population genetics (i.e., [3, 8]).

The purpose of the present paper is to find solutions to the regular case employing the powerful properties of Chebyshev polynomials coupled with sparse matrix routines. We assume that the reader is familiar with the general properties of these

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ISSN 0021-9991

polynomials; especially useful references are Fox and Parker [5], Snyder [14], and Rivlin [12]. We defer any discussion of these orthogonal polynomials until Section 2 and proceed to the formulation of the problem.

The Fokker–Planck (forward Kolmogorov) equation describing the time evolution of the transition probability $f(x, t \mid x_0, 0)$ is

$$\frac{\partial f}{\partial t} = \frac{1}{2} \frac{\partial^2}{\partial x^2} (Vf) - \frac{\partial}{\partial x} (Mf), \tag{1.1}$$

where $V(x)$, $M(x)$ are the infinitesimal transition moments

$$V(x) = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int (y - x)^2 f(y, \Delta t \mid x, 0)\, dy, \tag{1.2}$$

$$M(x) = \lim_{\Delta t \to 0} \frac{1}{\Delta t} \int (y - x) f(y, \Delta t \mid x, 0)\, dy. \tag{1.3}$$

Both M and V are assumed to be such that they do not vanish simultaneously at both boundaries.

Equation (1.1) is to be solved subject to the initial condition

$$\lim_{t \to 0} f(x, t \mid x_0, 0) = \delta(x - x_0) \tag{1.4}$$

as well as specified boundary conditions.

The boundary conditions are

$$f(x, t \mid x_0, 0) = 0, \qquad \text{for } \textit{absorbing} \text{ barrier}, \tag{1.5}$$

$$\tfrac{1}{2}(\partial/\partial x)(Vf) - Mf = 0, \qquad \text{for } \textit{reflecting} \text{ barrier}. \tag{1.6}$$

These boundary conditions will be taken at either (1) $x = \pm a$ or (2) $x = 0, a$; here a is taken to be finite. We can always scale the variables so that the intervals reduce to (1) $x = \pm 1$ or (2) $x = 0, 1$. We will treat both cases with special emphasis on case (2).

The analysis will be carried out for general $M(x)$ and $V(x)$, however, illustrative numerical calculations are performed for two important cases: the Wiener process with drift, and the Ornstein–Uhlenbeck process.

A quantity of considerable interest when one or both of the boundaries is absorbing is the probability density function of the first passage time $g(t, x_0)$ given by

$$g(t, x_0) = -\frac{d}{dt} \int f(x, t \mid x_0, 0)\, dx, \tag{1.7}$$

where the integration is either $(-a, a)$ or $(0, a)$. One of the chief benefits of the Chebyshev polynomial approach is the relative ease in evaluating $g(t, x_0)$. See Section 10 for some numerical results.

2. Chebyschev Approximation for Transition PDF

For typographic convenience set

$$f(x, t \mid x_0, 0) \equiv f(x, t). \tag{2.1}$$

We seek a solution of Eq. (1.1) in the form

$$f(x, t) = \sum_{n=0}^{N} A_n(t)\, T_n(x), \tag{2.2}$$

where $T_n(x)$ is the Chebyschev polynomial of degree n

$$T_n(x) = \cos(n \arccos x), \qquad |x| \leqslant 1. \tag{2.3}$$

The time-dependent function $A_n(t)$ is taken to be

$$A_n(t) = \sum_{r=0}^{R} a_{n,r} e^{\lambda_r t}, \tag{2.4}$$

where the $a_{n,r}$ are to be determined.

The behavior of the (as yet unknown) eigenvalues λ_r depends on the boundary conditions imposed. If *both* boundaries are taken to be *reflecting*, then the λ_r are nonpositive with one eigenvalue equal to zero. This guarantees a steady-state solution $f(x, \infty \mid x_0, 0)$ independent of the initial conditions such that

$$\int_0^1 f(x, t \mid x_0, 0)\, dx = 1, \qquad 0 \leqslant t \leqslant \infty. \tag{2.5}$$

However, when *one* (or *both*) of the boundaries is *absorbing*, then $f(x, t \mid x_0, 0)$ is no longer a probability density function. Now $f(x, t \mid x_0, 0)\, dx$ is to be interpreted as the probability that the random process $X(t)$, having started at $X(0) = x_0$, reaches a value between x and $x + dx$ at t. Consequently,

$$\lim_{t\to\infty} f(x, t \mid x_0, 0) = 0, \tag{2.6}$$

since absorption is bound to take place. This implies that *all* the λ_r are nonpositive.

The drift coefficients M and V are also to be expanded into a Chebyschev series

$$V(x) = \sum_n V_n T_n(x), \tag{2.7}$$

$$M(x) = \sum_n M_n T_n(x). \tag{2.8}$$

When M and V are polynomials in x, a very common occurrence, then these series are finite. However, if M or V are trigonometric functions, such as occur in phase-locked loops, Josepheson junctions, etc., then these series are infinite series.

Our problem naturally divides into two parts: the determination of the eigenvalues λ_r and the determination of the $a_{n,r}$ coefficients for the specified boundary conditions. These topics are the subjects of the next sections.

The Chebyschev expansion, Eq. (2.2), possesses the important property that it converges very rapidly (in the following sense). Suppose that $f(x, t)$ is infinitely differentiable for $t > 0$ (this is a reasonable statement since the Fokker–Planck equation, being a parabolic differential equation, will smooth out discontinuities); then the errors decrease more rapidly than any power of N^{-1} as N approaches infinity. A formal proof can be found in Orszag [11]. Thus the Chebyschev approach is efficient, in addition to having other useful properties.

3. Solution for $(-1, +1)$

We now express Eq. (1.1) in terms of Chebyschev polynomials and thereby obtain coupled differential equations connecting the eigenvalues λ_r and the $a_{n,r}$ coefficients. The analysis proceeds in three steps:

Step 1. Expansion of $(Vf)_{xx}$. Let

$$Vf = \sum_p R_p^{(0)} T_p(x). \tag{3.1}$$

By Eq. (A.8), we have

$$\bar{R}_p^{(0)} = \tfrac{1}{2} \sum_{m=-\infty}^{\infty} \bar{V}_{|p-m|} \bar{A}_{|m|}(t). \tag{3.2}$$

Now let

$$(Vf)_{xx} = \sum_n R_n^{(2)} T_n(x). \tag{3.3}$$

By Eq. (A.5) we have

$$\begin{aligned} \bar{R}_n^{(2)} &= \sum_{\substack{p=n+2 \\ p\equiv n (\mathrm{mod}\ 2)}}^{\infty} p(p^2 - n^2)\, R_p^{(0)} \\ &= \tfrac{1}{2} \sum_{m=-\infty}^{\infty} \bar{A}_{|m|}(t) \cdot \sum_{\substack{p=n+2 \\ p\equiv n (\mathrm{mod}\ 2)}}^{\infty} c_p^{-1} p(p^2 - n^2)\, \bar{V}_{|p-m|}\,. \end{aligned} \tag{3.4}$$

Step 2. Expansion of $(Mf)_x$. Let

$$Mf = \sum_p S_p^{(0)} T_p(x). \tag{3.5}$$

By Eq. (A.8), we have

$$\bar{S}_p^{(0)} = \tfrac{1}{2} \sum_{m=-\infty}^{\infty} \bar{M}_{|p-m|} \bar{A}_{|m|}(t). \tag{3.6}$$

Now let the derivative of Mf be

$$(Mf)_x = \sum_n S_n^{(1)} T_n(x). \tag{3.7}$$

By Eq. (A.1), we obtain

$$\begin{aligned} \bar{S}_n^{(1)} &= 2 \sum_{\substack{p=n+1 \\ |p+n| \equiv 1 (\mathrm{mod}\ 2)}}^{\infty} p S_p^{(0)} \\ &= \sum_{m=-\infty}^{\infty} \bar{A}_{|m|}(t) \cdot \sum_{\substack{p=n+1 \\ |p+n| \equiv 1 (\mathrm{mod}\ 2)}}^{\infty} p \bar{M}_{|p-m|}. \end{aligned} \tag{3.8}$$

Step 3. Eigenvalue differential equation. Let

$$K(m, n) = \tfrac{1}{4} \sum_{\substack{p=n+2 \\ p \equiv n (\mathrm{mod}\ 2)}}^{\infty} p(p^2 - n^2)\, \bar{V}_{|p-m|} - \sum_{\substack{p=n+1 \\ |p+n| \equiv 1 (\mathrm{mod}\ 2)}}^{\infty} p \bar{M}_{|p-m|}. \tag{3.9}$$

We then have

$$\begin{aligned} (d/dt)\, A_n(t) &= \sum_{m=-\infty}^{\infty} \bar{A}_m(t)\, K(m, n) \\ &= \sum_{m=0}^{\infty} A_m(t)[K(m, n) + K(-m, n)]. \end{aligned} \tag{3.10}$$

Upon expanding the right-hand side of this equation, we can show that

$$\lambda_r a_{n,r} = \sum_{m=0}^{\infty} a_{m,r}[K(m, n) + K(-m, n)]. \tag{3.11}$$

This infinite system partially determines the eigenvalues, but of course only a finite section can be employed in actual calculations. If the upper limit is taken as N, then Eq. (3.11) furnishes $N + 1$ equations.

Equation (3.11) by itself is useless and we need to impose the boundary conditions and the initial conditions. The initial conditions are easily handled, so we have[1]

$$f(x, 0) = \delta(x - x_0) = \sum_{n=0}^{N} A_n(0)\, T_n(x), \tag{3.12}$$

where

$$\begin{aligned} A_n(0) &= \int_{-1}^{+1} \frac{1}{c_n}\, \delta(x - x_0)(1 - x^2)^{-1/2}\, T_n(x)\, dx \\ &= \frac{2}{\pi c_n} (1 - x_0^2)^{-1/2}\, T_n(x_0), \end{aligned} \tag{3.13}$$

where c_n is defined as

$$\begin{aligned} c_n &= 0, \qquad n < 0, \\ &= 2, \qquad n = 0, \\ &= 1, \qquad n > 0. \end{aligned} \tag{3.14}$$

Consequently,

$$\sum_{r=0}^{R} a_{n,r} = [2/(\pi c_n)](1 - x_0^2)^{-1/2}\, T_n(x_0) \equiv \beta_n'(x_0) \tag{3.15}$$

for $n = 0, 1, \ldots$.

For an *absorbing* boundary at $x = 1$, we have

$$f(1, t) = \sum_{n=0}^{N} A_n(t) = 0, \tag{3.16}$$

since $T_n(1) = 1$; this translates into the requirement

$$\sum_{n=0}^{N} a_{\;,r} = 0. \tag{3.17}$$

The corresponding expression for an absorbing boundary at $x = -1$ is

$$\sum_{n=0}^{N} (-1)^n\, a_{n,r} = 0. \tag{3.18}$$

Note that $T_n(-1) = (-1)^n$.

The formulas for a *reflecting* barrier are more complicated. Set

$$C(m, n) = \tfrac{1}{2} \sum_{\substack{p=n+1 \\ |p+n| \equiv 1 (\mathrm{mod}\ 2)}}^{\infty} p \overline{V}_{|p-m|} - \tfrac{1}{2} \overline{M}_{|m-n|}\, . \tag{3.19}$$

[1] We approximated the Dirac delta function in Eq. (3.12) by a Gaussian PDF having mean x_0 and very small variance σ^2.

At $x = 1$, we can show that

$$0 = \sum_{m=0}^{\infty} a_{m,r} \sum_{n=0}^{\infty} [C(m, n) + C(-m, n)], \tag{3.20}$$

while at $x = -1$,

$$0 = \sum_{m=0}^{\infty} a_{m,r} \sum_{n=0}^{\infty} (-1)^n [C(m, n) + C(-m, n)]. \tag{3.21}$$

4. Solution for (0, +1)

This analysis is similar to that of the previous sections, except that we employ the shifted Chebyschev polynomials $T_n^*(x)$,

$$T_n^*(x) = T_n(2x - 1), \qquad 0 \leqslant x \leqslant 1. \tag{4.1}$$

Here we have

$$f(x, t) = \sum_{n=0}^{N} A_n^*(t)\, T_n^*(x), \tag{4.2}$$

where

$$A_n^*(t) = \sum_{r=0}^{R} a_{n,r}^* e^{\lambda_r t}. \tag{4.3}$$

By methods similar to those just employed, we can prove that the eigenvalue differential equation corresponding to Eq. (3.11) is

$$\lambda_r a_{n,r}^* = \sum_{m=0}^{\infty} a_{m,r}^* [K^*(m, n) + K^*(-m, n)], \tag{4.4}$$

where

$$K^*(m, n) = \sum_{\substack{p=n+2 \\ p\equiv n (\mathrm{mod}\ 2)}}^{\infty} p(p^2 - n^2)\, \overline{V}_{|p-m|} - 2 \sum_{\substack{p=n+1 \\ |p+n| \equiv 1 (\mathrm{mod}\ 2)}}^{\infty} p\widetilde{M}_{|p-m|}\,. \tag{4.5}$$

The formula corresponding to Eq. (3.15) for the initial condition is

$$\sum_{r=0}^{R} a_{n,r}^* = \frac{T_n^*(x_0)}{\pi c_n (x_0 - x_0^2)^{1/2}} \equiv \beta_n(x_0). \tag{4.6}$$

The boundary conditions are handled in much the same manner.

The final results for an *absorbing* boundary at $x = 0$ and $x = 1$ are

$$\sum_{n=0}^{N} (-1)^n a_{n,r}^* = 0, \tag{4.7}$$

$$\sum_{n=0}^{N} a_{n,r}^* = 0. \tag{4.8}$$

The corresponding expressions for a *reflecting* boundary at $x = 0$ and $x = 1$ are

$$\sum_{m=0}^{N} a_{m,r}^* \sum_{n=0}^{\infty} (-1)^n [C^*(m, n) + C^*(-m, n)] = 0, \tag{4.9}$$

$$\sum_{m=0}^{N} a_{m,r}^* \sum_{n=0}^{\infty} [C^*(m, n) + C^*(-m, n)] = 0, \tag{4.10}$$

where

$$C^*(m, n) = \sum_{\substack{p=n+1 \\ |p+n| \equiv 1 (\mathrm{mod}\ 2)}}^{\infty} p\overline{V}_{|p-m|} - \tfrac{1}{2}\overline{M}_{|m-n|}\,. \tag{4.11}$$

5. Determination of the Eigenvalues

In order to determine the eigenvalues, we employ Eq. (3.11) or Eq. (4.4), depending on the fundamental interval in question. Either equation furnishes a system of $N + 1$ equations for the determination of the eigenvalues. In addition, there are two equations for the boundary conditions:

$$\sum_{m=0}^{N} A_m{}^*(t)\, b_m^{(1)} = \sum_{m=0}^{N} A_m{}^*(t)\, b_m^{(2)} = 0, \tag{5.1}$$

where

$$\begin{aligned} b_m^{(1)} &= 1 && \text{(the absorbing boundary),} \\ &= \sum_{m=0}^{\infty} [C^*(m, n) + C^*(-m, n)] && \text{(the reflecting boundary),} \end{aligned} \tag{5.2}$$

at $x = 1$, and

$$\begin{aligned} b_m^{(2)} &= (-1)^m && \text{(the absorbing boundary),} \\ &= \sum_{m=0}^{\infty} (-1)^m [C^*(m, n) + C^*(-m, n)] && \text{(the reflecting boundary),} \end{aligned} \tag{5.3}$$

at $x = 0$. Henceforth we confine ourselves to $(0, 1)$; the $(-1, 1)$ interval can be treated similarly.

The system of equations is overdetermined by 2 and admits only the trivial solution. Therefore we must resort to the tau method of Lanczos [9] and add two tau terms in the two highest-order equations. This corresponds to the elimination of the two highest-order terms of the expansion, so we are left with $N+1$ equations. The eigenvalues can now be determined by the standard QR algorithm in time $O(N^3)$, as discussed in [16].

6. Determination of $a_{n,r}$ Coefficients

This section is devoted to methods for determining the $a_{n,r}$ coefficients. We again confine the analysis to (0, 1). As in the previous section, we drop the two highest-order terms of the Chebyschev expansion, Eq. (4.4), so as to satisfy the boundary conditions. Equations (5.1) translate into

$$\sum_{m=0}^{N} a_{m,r}^* b_m^{(1)} = \sum_{m=0}^{N} a_{m,r}^* b_m^{(2)} = 0. \tag{6.1}$$

Thus we have $(N+1)\cdot(R+1)$ equations; however, we must also add the equations for the initial conditions

$$\sum_{r=0}^{R} a_{n,r}^* = \beta_n(x_0), \qquad n = 0, 1,..., N, \tag{4.6}$$

which means we really have $(N+1)\cdot(R+2)$ equations. Since we only need $(N+1)\cdot(R+1)$ coefficients, the system is overdetermined by $N+1$ equations. Again we resort to the tau method of Lanczos for $r = 0, 1,..., R$. Equation (4.4) now becomes

$$\sum_{m=0}^{N} a_{m,r}^*[K^*(m, n) + K^*(-m, n)] - \lambda_r a_{n,r}^* = \mu_{n,r}, \tag{6.2}$$

where $n = 0, 1,..., N-2$, and $\mu_{n,r}$ is defined to be

$$\begin{aligned} \mu_{n,r} &= \tau_r, && \text{for } n = N-2 \textit{ and } r = 0, 1,..., R-1,\\ &= \tau_n, && \text{for } n = R-2,..., N-2 \textit{ and } r = R,\\ &= 0, && \text{elsewhere.} \end{aligned} \tag{6.3}$$

Note that the $(N+1)$ tau terms are added in such a manner so as to preserve the boundary conditions. Now we have $(N+1)\cdot(R+1)$ equations and the same number of unknowns. A naive solution requires $O(R^3N^3)$ time and $O(R^2N^2)$ space.

Note that the resultant system of linear equations has a very sparse structure (see Fig. 1). We now present a method which efficiently exploits the sparsity structure of the system and requires only $O(RN^3)$ time and $O(N^2)$ space. See [13, 17] for details

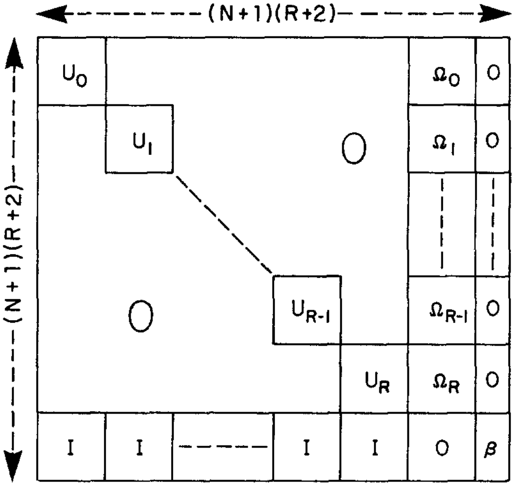

FIG. 1. Diagram of the sparsity structure of the system of equations where $\hat{I}$ is an $(N+1)(N+1)$ unit matrix and $\hat{\Omega}_r$ is an $(N+1)(N+1)$ matrix:

$$\begin{aligned} \Omega_r(m,n) &= 1, \quad n = N-2, \quad 0 \leqslant r < R, \\ &= 1, \quad r = R, \quad R-2 \leqslant n \leqslant N-2, \\ &= 0, \quad \text{elsewhere.} \end{aligned}$$

$\hat{U}_r$ is an $(N+1)(N+1)$ matrix:

$$\begin{aligned} U_r(m,n) &= [K^*(m,n) + K^*(-m,n)], \quad m \neq n = 0,\ldots, N-2 \\ &= [K^*(m,n) + K^*(-m,n)] - \lambda_r \quad m = n = 0,\ldots, N-2 \\ &= b_m^{(1)}, \quad n = N-1, \\ &= b_m^{(2)}, \quad n = N. \end{aligned}$$

$\hat{\beta}$ is a column matrix composed of $\beta_0, \ldots, \beta_N$.

of the analysis. Our strategy is *not* to solve for the $a_{n,r}$ unknowns directly, but instead to first determine the tau terms and then back-solve for the $a_{n,r}$. This process requires three steps:

1. *Determination of the a^* terms in relation to the τ terms.* For each $r = 0, 1,\ldots, R$ we must determine the coefficients $\alpha_{0,r}^* \cdots \alpha_{N,r}^*$, where

$$\begin{aligned} a_{n,r}^* &= \alpha_{n,r}^* \tau_r, \quad \begin{cases} r = 0, 1,\ldots, R-1, \\ n = 0, 1,\ldots, N; \end{cases} \\ &= \sum_{r=R}^{N} \alpha_{n,r}^* \tau_r, \quad n = 0, 1,\ldots, N. \end{aligned} \tag{6.4}$$

This step requires $O(RN^3)$ time. Since each $\alpha_{0,r}^* \cdots \alpha_{N,r}^*$ are determined separately for each r, only $O(N^2)$ space is required for this step.

2. *Solving for the τ terms.* Now substituting Eq. (6.4) into the equations for the initial conditions, we have

$$\sum_{r=0}^{N} \alpha_{n,r}^{*}\tau_r = \beta_n(x_0), \qquad n = 0, 1,..., N. \tag{6.5}$$

The τ terms can be determined in $O(N^3)$ time.

3. *Backsolve for the $a_{n,r}^{*}$ coefficients.* Now that the τ coefficients have been determined, the $a_{n,r}^{*}$ coefficients can be determined in $O(RN^2)$ time by the relations computed in Step 1. This three step process requires $O(RN^3)$ time and $O(N^2)$ space.

7. First Passage Time PDF

The first passage time PDF, $g(t, x_0)$, given by Eq. (1.7), is easily evaluated. We confine our attention to the evaluation of $g(t, x_0)$ for the interval (0, 1).

Upon substituting Eq. (4.2) into Eq. (1.7), we obtain

$$g(t, x_0) = -\sum_{n=0}^{N} A_n'^{*}(t)\, h_n , \tag{7.1}$$

where

$$A_n'^{*} = \sum_{r=0}^{R} a_{n,r}^{*}\lambda_r e^{\lambda_r t} \tag{7.2}$$

and

$$\begin{aligned} h_n &\equiv \int_0^1 T_n^{*}(x)\, dx \\ &= 1, && n = 0, \\ &= 0, && n = 1, \\ &= \frac{1}{4}\left[\frac{T_{n+1}^{*}(x)}{n+1} - \frac{T_{n-1}^{*}(x)}{n-1}\right], && n > 1. \end{aligned} \tag{7.3}$$

The simple expression for $g(t, x_0)$ given in Eq. (7.1) permits its calculation as part of the evaluation of $f(x, t \mid x_0, 0)$ or independently.

8. Numerical Results: Wiener Process

For the Wiener process with drift, the derivate moments are

$$V = 2D, \qquad M = 4\beta D, \tag{8.1}$$

where D and β are numerical constants (see [2]). We will convert to dimensionless variables by setting $x_1 = x/a$, $t_1 = Dt/a^2$, and $\beta_1 = a\beta$. The Fokker–Planck equation becomes

$$\frac{\partial f}{\partial t_1} = -4\beta_1 \frac{\partial^2 f}{\partial x_1^2} + \frac{\partial f}{\partial x_1}, \qquad 0 < x_1 < 1. \tag{8.2}$$

The corresponding equations for the boundary conditions are

$$\frac{\partial f}{\partial x_1} - 4\beta_1 f = 0, \qquad x_1 = 0 \text{ or } 1 \tag{8.3}$$

at a reflecting barrier and $f = 0$ at $x_1 = 0$ or 1 at an absorbing barrier.

There are four cases to consider:

1. RR: reflecting at $x = 0$, reflecting at $x = 1$;
2. AA: absorbing at $x = 0$, absorbing at $x = 1$;
3. AR: absorbing at $x = 0$, reflecting at $x = 1$;
4. RA: reflecting at $x = 0$, absorbing at $x = 1$.

In case RR, the transient solution $f(x_1, t_1)$ approaches the steady-state solution

$$f(x_1, \infty) = 4\beta_1(e^{4\beta_1} - 1)^{-1} e^{4\beta_1 x_1}, \tag{8.4}$$

which arises from the fact that one of the eigenvalues of Eq. (8.2) is zero. Here $f(x_1, t_1)$ is a true probability density function. The remaining three cases all have absorbing boundaries and any process confined between them will ultimately be absorbed, i.e.,

$$f(x_1, \infty) = 0. \tag{8.5}$$

For these cases, $f(x_1, t_1)$ is to be understood to mean the probability density that the random process $X(t) = x$ and that the process has not yet reached the boundaries in $(0, t_1)$.

We have made no serious attempt to develop a detailed catalog of numerical results and we confine our presentation to a few typical results. In the calculations which follow, and for those of the next section also, we employed 20 eigenvalues and 27 coefficients and took the Dirac delta function to be centered at $x_0 = 0.5$. The drift coefficient was fixed at $\beta_1 = 0.125$.

Numerical results for the RR case are summarized in Fig. 2. Note how rapidly the transient solution approaches the steady-state solution. The numerical results for the AA case are shown in Fig. 3; the curves are not symmetric about $x_0 = 0.5$ since $\beta_1 > 0$. Finally, the curves for the AR case are displayed in Fig. 4; the corresponding curves for the RA case are essentially mirror images of the AR case (at least for $\beta_1 = 0.125$). There is a fairly slow relaxation of the initial Dirac delta function to the limiting value of zero. We also ran some calculations for an off-center Dirac

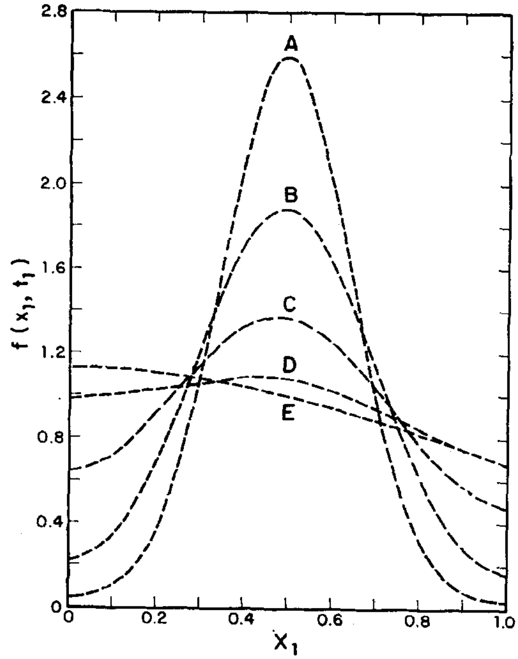

FIG. 2. $f(x_1, t_1)$ for Wiener process with reflecting boundaries at $x_1 = 0, 1$ ($\beta_1 = 0.125$, $x_0 = 0.50$): (A) $t_1 = 0.01$; (B) $t_1 = 0.02$; (C) $t_1 = 0.04$; (D) $t_1 = 0.08$; (E) $t_1 = \infty$.

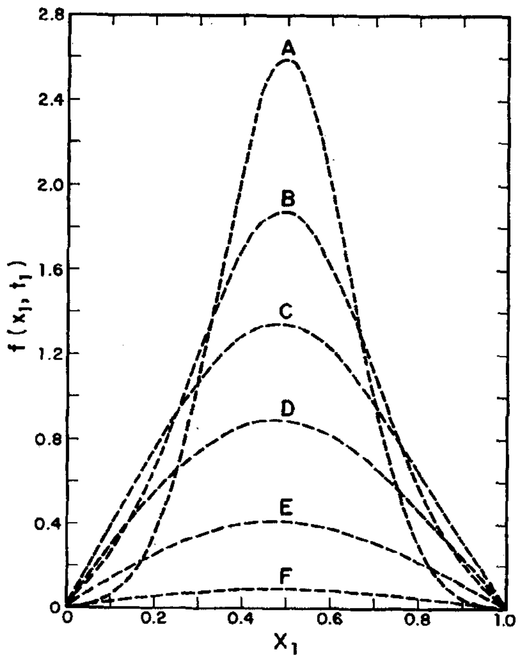

FIG. 3. $f(x_1, t_1)$ for Wiener process with absorbing boundaries at $x_1 = 0, 1$ ($\beta_1 = 0.125$, $x_0 = 0.50$): (A) $t_1 = 0.01$; (B) $t_1 = 0.02$; (C) $t_1 = 0.04$; (D) $t_1 = 0.08$; E) $t_1 = 0.16$; (F) $t_1 = 0.32$.

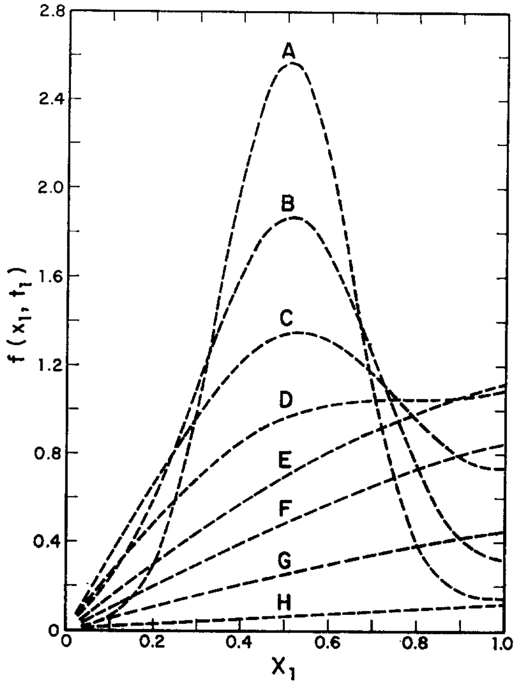

FIG. 4. $f(x_1, t_1)$ for Wiener process with absorbing boundary at $x_1 = 0$ and reflecting boundary at $x_1 = 1$ ($\beta_1 = 0.125$, $x_0 = 0.50$): (A) $t_1 = 0.01$; (B) $t_1 = 0.02$; (C) $t_1 = 0.04$; (D) $t_1 = 0.08$; (E) $t_1 = 0.16$; (F) $t_1 = 0.32$; (G) $t_1 = 0.64$; (H) $t_1 = 1.28$.

delta function (i.e., $x_0 \neq 0.5$). It appears that the approach to the equilibrium situation is strongly influenced by the degree to which x_0 differs from 0.5; the "decay" times are much longer.

9. Numerical Results, Ornstein–Uhlenbeck Process

For the Ornstein–Uhlenbeck process, the derivate moments are

$$V = 2D, \qquad M = -\alpha x, \qquad \alpha > 0. \tag{9.1}$$

The corresponding Fokker–Planck equation can be cast into dimensionless form by setting $x_1 = x/a$, $t_1 = Dt/a^2$, and $\alpha_1 = a^2\alpha/D$; thus

$$\frac{\partial f}{\partial t_1} = \frac{\partial^2 f}{\partial {x_1}^2} + \alpha_1 \frac{\partial (x_1 f)}{\partial x_1} \qquad (0 < x_1 < 1). \tag{9.2}$$

The boundary condition for a reflecting barrier is

$$\frac{\partial f}{\partial x_1} + \alpha_1 x_1 f = 0, \qquad x_1 = 0 \text{ or } 1. \tag{9.3}$$

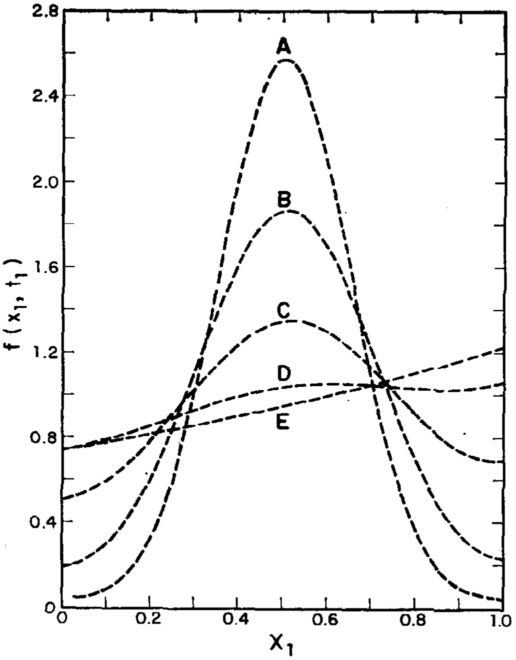

FIG. 5. $f(x_1, t_1)$ for OU process with reflecting boundaries at $x_1 = 0, 1$ ($\alpha_1 = 1$, $x_0 = 0.50$): (A) $t_1 = 0.01$; (B) $t_1 = 0.02$; (C) $t_1 = 0.04$; (D) $t_1 = 0.08$; (E) $t_1 = \infty$.

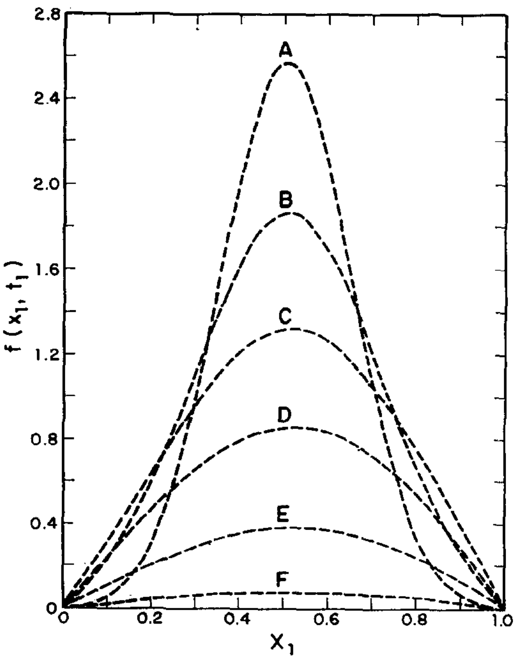

FIG. 6. $f(x_1, t_1)$ for OU process with absorbing boundaries at $x_1 = 0, 1$ ($\alpha_1 = 1$, $x_0 = 0.50$): (A) $t_1 = 0.01$; (B) $t_1 = 0.02$; (C) $t_1 = 0.04$; (D) $t_1 = 0.8$; (E) $t_1 = 0.16$; (F) $t_1 = 0.32$.

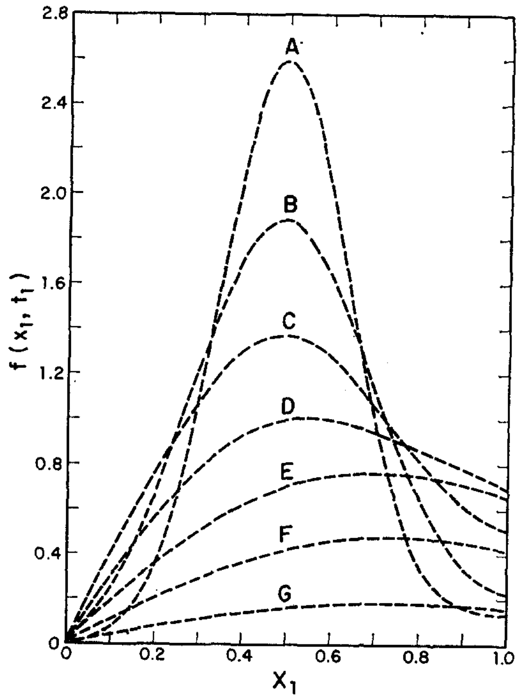

FIG. 7. $f(x_1, t_1)$ for OU process with absorbing boundary at $x_1 = 0$ and reflecting boundary at $x_1 = 1$ ($\alpha_1 = 1$, $x_0 = 0.50$): (A) $t_1 = 0.01$; (B) $t_1 = 0.02$; (C) $t_1 = 0.04$; (D) $t_1 = 0.08$; (E) $t_1 = 0.16$; (F) $t_1 = 0.32$; (G) $t_1 = 0.64$.

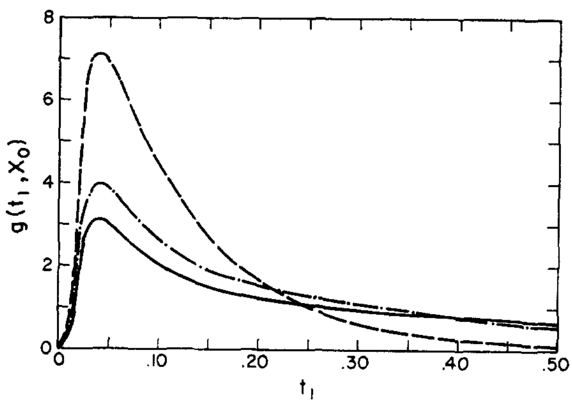

FIG. 8. $g(t_1, x_0)$ for Wiener process ($\beta_2 = 0.125$, $x_0 = 0.50$) for various boundary conditions: --- AA, — · — RA, ——— AR.

The corresponding numerical calculations are shown in Figs. 5–7 and do not require any detailed comment. Note that $\alpha_1 = 1$ for these calculations.

During the revision of this manuscript, the important paper of Lindenberg, Schuler, Freeman, and Lie [10] on the Ornstein–Uhlenbeck process has appeared.

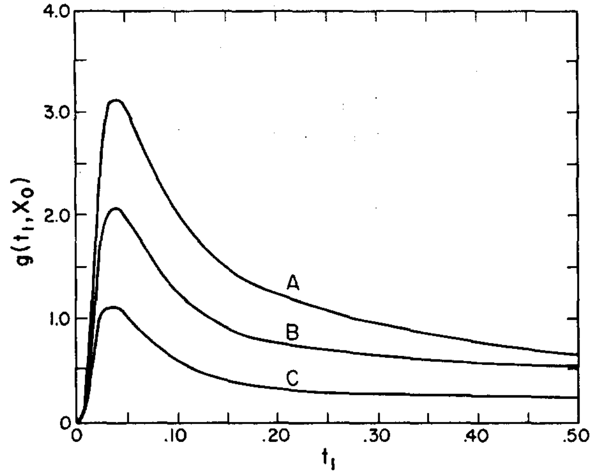

FIG. 9. $g(t_1, x_0)$ for Wiener process for absorbing–reflecting boundaries as a function of $\beta_1(x_0 = 0.50)$: (A) $\beta_1 = 0.125$; (B) $\beta_1 = 0.50$; (C) $\beta_1 = 2.0$.

10. FIRST PASSAGE TIME PDF'S

The first passage time PDF $g(t_1, x_0)$, Eq. (7.1), was also evaluated for the Wiener and Ornstein–Uhlenbeck processes. As before, 20 eigenvalues and 27 Chebyschev coefficients were employed.

TABLE I

First Six Eigenvalues, Wiener Process with Drift With $\beta_1 = 0.125$, for Various Boundary Conditions at $x = 0, 1$

	AA	AR	RA	RR
$-\lambda_0$	0.993210(01)	0.200364(01)	0.300547(01)	0
$-\lambda_1$	0.395409(02)	0.217667(02)	0.227659(02)	0.993210(01)
$-\lambda_2$	0.888889(02)	0.612467(02)	0.622464(02)	0.395409(02)
$-\lambda_3$	0.157976(03)	0.120465(03)	0.121465(03)	0.888889(02)
$-\lambda_4$	0.246803(03)	0.199422(03)	0.200422(03)	0.157976(03)
$-\lambda_5$	0.355368(03)	0.298118(03)	0.299118(03)	0.246803(03)

The calculations for the Wiener process are summarized in Figs. 8 and 9. In Fig. 8, we show $g(t_1, x_0)$ for fixed $\beta_1 = 0.125$, $x_0 = 0.5$ for various combinations of boundary conditions. As expected, the absorbing–absorbing case tends to zero, as t_1 increases much more rapidly than the other cases. The rate at which $g(t_1, x_0)$ tends to zero is governed by the first eigenvalue. Examination of Table I reveals that the absorbing–reflecting case has the smallest eigenvalue and hence the slowest rate of decay. Figure 9 illustrates the behavior of $g(t_1, x_0)$ for the absorbing–reflecting case as a function of β_1. The larger the drift coefficient β_1, the slower the decay to zero as a function of t_1. This accords with the numerical calculations.

The corresponding calculations for the Ornstein–Uhlenbeck process are given in

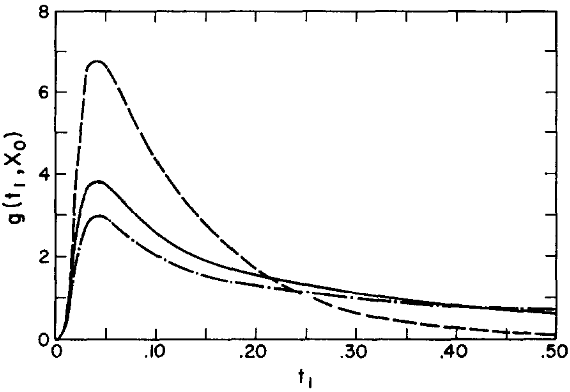

FIG. 10. $g(t_1, x_0)$ for Ornstein–Uhlenbeck process ($\alpha_1 = 1.0$, $x_0 = 0.50$) for various boundary conditions: --- AA, — · — RA, ——— AR.

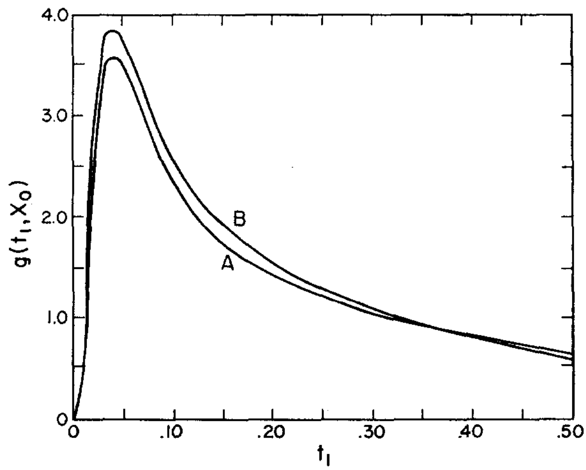

FIG. 11. $g(t_1, x_0)$ for Ornstein–Uhlenbeck process for absorbing–reflecting boundaries as a function of $\alpha_1(x_0 = 0.50)$: (A) $\alpha_1 = 0.125$; (B) $\alpha_1 = 1.0$.

Figs. 10 and 11. Note that the reflecting–absorbing case now has the slowest rate of decay (see Table II). The absorbing–reflecting case, Fig. 11, is quite interesting in that it shows how insensitive is $g(t_1, x_0)$ to the coefficient α_1.

TABLE II

First Six Eigenvalues, Ornstein–Uhlenbeck Process with $\alpha_1 = 1$, for Various Boundary Conditions at $x = 0, 1$

	AA	AR	RA	RR
$-\lambda_0$	0.944020(01)	0.300000(01)	0.200000(01)	0
$-\lambda_1$	0.390586(02)	0.227843(02)	0.217843(02)	0.104402(02)
$-\lambda_2$	0.884084(02)	0.622664(02)	0.612664(02)	0.400586(02)
$-\lambda_3$	0.157496(03)	0.121485(03)	0.120485(03)	0.894084(02)
$-\lambda_4$	0.246323(03)	0.200442(03)	0.199442(03)	0.158496(03)
$-\lambda_5$	0.354889(03)	0.299139(03)	0.298139(03)	0.247323(03)

There is no difficulty in also obtaining such items as the mean of the first passage time, etc. Obviously such functions must be evaluated over a variety of parameter values, times, boundary conditions, etc., if they are to be useful. However, such detailed calculations are outside the spirit of the present paper and we hope that some interested reader can undertake this task.

Appendix

In this Appendix we list some important formulas which are crucial for the analysis outlined in Sections 3 and 4 (see [5] for details).

It is convenient to define a function

$$\begin{aligned} c_n &= 0, \qquad n < 0, \\ &= 2, \qquad n = 0, \\ &= 1, \qquad n > 0. \end{aligned} \tag{A.1}$$

Let the function $F(x)$ be expanded in a Chebyschev series in the interval $(-1, 1)$

$$F(x) = \sum_{n=0}^{\infty} a_n T_n(x). \tag{A.2}$$

Provided the jth derivative of $F(x)$ exists, we can also write

$$d^jF/dx^j = \sum_{n=0}^{\infty} a_n^{(j)} T_n(x). \tag{A.3}$$

The relation between the coefficients of these two series is discussed in Fox and Parker; in the notation of Orszag [11], the pertinent relations are

$$a_n^{(1)} = \frac{2}{c_n} \sum_{\substack{p=n+1 \\ (p+n)\equiv 1 (\mathrm{mod}\ 2)}} p a_p , \qquad n \geqslant 0, \tag{A.4}$$

$$a_n^{(2)} = \frac{1}{c_n} \sum_{\substack{p=n+2 \\ p\equiv n (\mathrm{mod}\ 2)}} p(p^2 - n^2)\, a_p , \qquad n \geqslant 0, \tag{A.5}$$

where $a \equiv b$ (mod 2) means that $(a - b)$ is divisible by 2.

Now consider the product of two functions $G(x)$, $F(x)$, where $F(x)$ has the expansion, Eq. (A.2), and $G(x)$ has the expansion

$$G(x) = \sum_{n=0}^{\infty} b_n T_n(x). \tag{A.6}$$

We have

$$G(x) F(x) = \sum_{n=0}^{\infty} e_n T_n(x). \tag{A.7}$$

It is possible to prove that

$$\bar{e}_n \equiv c_{|n|} e_{|n|} = \tfrac{1}{2} \sum_{p=-\infty}^{\infty} \bar{a}_{|p-n|} \bar{b}_{|p|} , \tag{A.8}$$

where $\bar{a}_n \equiv c_{|n|} a_{|n|}$, $\bar{b}_n \equiv c_{|n|} b_{|n|}$.

We will also need the corresponding formulas for the interval (0, 1). In order to do this, we simply replace $T_n(x)$ by the shifted Chebyschev polynomial $T_n{}^*(x)$. The companion results to Eqs. (A.4), (A.5), and (A.8) are

$$a_n^{(1)} = 4 \sum_{\substack{p=n+1 \\ |p+n|\equiv 1 (\mathrm{mod}\ 2)}} p a_p , \tag{A.9}$$

$$a_n^{(2)} = 4 \sum_{\substack{p=n+2 \\ p\equiv n (\mathrm{mod}\ 2)}} p(p^2 - n^2)\, a_p , \tag{A.10}$$

$$\bar{e}_n = \tfrac{1}{2} \sum_{p=-\infty}^{\infty} \bar{a}_{|p-n|} \bar{b}_{|p|} .$$

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