Journal of Statistical Physics, Vol. 66, Nos. 5/6, 1992

First Passage Time Distribution in an Oscillating Field

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Received May 3, 1991; final October 29, 1991

Siegert's integral equation approach to calculate the first passage time distribution is generalized to the case of a one-dimensional diffusion process in an oscillating drift field. A simple algorithm to solve the integral equations is developed and numerical results are presented.

KEY WORDS: Diffusion process; first passage time distribution; Fokker–Planck equation; Siegert integral equations.

Diffusive transport in an oscillating field is a useful model in analyzing experiments on the separation of large DNA molecules by pulsed fields.[1] A property of primary interest in such models is the mean first passage time a particle takes to exit from a specified spatial domain. Direct simulation of the transport or numerical treatment of the associated Fokker–Planck equation are methods usually employed to study first passage time problems in time-dependent fields.[1]

In this paper, we present a generalization of the Siegert integral equation theory[2] of first passage time problems to the case of a diffusion process in an oscillating field. We begin with the Fokker–Planck equation associated with one-dimensional diffusive transport[1]

$$\frac{\partial P}{\partial t} = -v(t)\frac{\partial P}{\partial x} + \frac{\partial^2 P}{\partial x^2} \tag{1}$$

where x and t are the dimensionless space and time variables and

$$v(t) = \varepsilon \sin(\omega t) \tag{2}$$

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0022-4715/92/0300-1675$06.50/0

is a sinusoidally varying drift field of amplitude ε and frequency ω. We are interested in calculating the first passage time distribution of the particle from the domain $[-1, 1]$. The standard formulation of the problem[3] is in terms of the probability $P(x, t)\,dx$ that the particle is in dx around x at time t and has not exited the domain earlier. $P(x, t)$ can be obtained[3] as the solution of Eq. (1) with the boundary conditions

$$P(\pm 1, t) = 0 \tag{3}$$

and any prescribed initial condition at $t = 0$. The cumulative probability $W_0(t)$ that the particle is in $[-1, 1]$ up to time t is

$$W_0(t) = \int_{-1}^{1} P(x, t)\,dx \tag{4}$$

and the first passage time distribution $g(t)$ is given by[3]

$$g(t) = -\frac{dW_0}{dt} \tag{5}$$

The boundary value problem of Eqs. (1) and (3) can be formulated[4] as an intgral equation using the infinite-medium Green's function (or conditional probability) $G(x, t \mid x', t')$. This formulation yields a representation for $P(x, t)$ as

$$\begin{aligned} P(x, t) = P_\infty(x, t) - \int_0^t [G(x, t \mid -1, t')\, P'(-1, t) \\ - G(x, t \mid 1, t')\, P'(1, t')]\, dt' \end{aligned} \tag{6}$$

for x in the domain $[-1, 1]$. The first term $P_\infty(x, t)\,dx$ represents the infinite-medium probability of finding the particle in dx around x at t and can be expressed as

$$P_\infty(x, t) = \int_{-1}^{1} G(x, t \mid x', 0)\, P_{\text{in}}(x')\, dx' \tag{7}$$

where $P_{\text{in}}(x')$ is the initial distribution (at $t = 0$) of the particle position. Under the integral sign in Eq. (6), $\mp P'(\pm 1, t)$ (where P' is the spatial derivative of P) in the integral terms in Eq. (6) denote the outward fluxes of particle trajectories at ± 1, since $P(\pm 1, t) = 0$ due to the boundary conditions. The physical interpretation of Eq. (6) is thus clear since the integral term is just the contribution to $P_\infty(x, t)$ of trajectories exited from $[-1, 1]$

prior to time t. The infinite-medium Green's function is a Gaussian function given by

$$G(x, t \mid x', t') = [4\pi(t-t')]^{-1/2} \exp\left\{-\frac{[x-x'-V(t, t')]^2}{4(t-t')}\right\} \tag{8}$$

where $V(t, t')$ is defined as

$$V(t, t') = \int_{t'}^{t} v(t'')\, dt'' = \frac{\varepsilon}{\omega} [\cos(\omega t') - \cos(\omega t)] \tag{9}$$

Several equivalent forms of Siegert's integral equations for $W_0(t)$ or $g(t)$ can now be derived[4] using the representation for $P(x, t)$ in Eq. (6). Indeed, integrating Eq. (1) over x (from -1 to 1) and using Eqs. (3)–(5), we get

$$\frac{dW_0}{dt} = P'(1, t) - P'(-1, t') \equiv -g(t) \tag{10}$$

In a similar way, the first spatial moment of $P(x, t)$, namely

$$W_1(t) = \int_{-1}^{1} xP(x, t)\, dx \tag{11}$$

is found to satisfy the relation

$$\frac{dW_1}{dt} = v(t)\, W_0 + P'(1, t) + P'(-1, t') \tag{12}$$

Taking the zeroth and first spatial moments (over the interval -1 to 1) of Eq. (6) and expressing $P'(\pm 1, t)$ in terms of dW_0/dt and dW_1/dt, we obtain the integral equations

$$\begin{aligned} W_k(t) = S_k(t) &+ \int_0^t G_k^+(t, t') \frac{dW_0}{dt'}\, dt' \\ &+ \int_0^t G_k^-(t, t') \left[\frac{dW_1}{dt'} - v(t')\, W_0(t')\right] dt', \qquad k = 0, 1 \end{aligned} \tag{13}$$

where the source functions $S_k(t)$ are given by

$$S_k(t) = \int_{-1}^{1} x^k P_\infty(x, t)\, dx, \qquad k = 0, 1 \tag{14}$$

and the kernel functions $G_k^{\pm}(t, t')$ by

$$G_k^{\pm}(t, t') = \frac{1}{2} \int_{-1}^{1} x^k [G(x, t \mid 1, t') \pm G(x, t \mid -1, t')] \, dx, \qquad k = 0, 1 \tag{15}$$

Equations (13) are a generalization of the Siegert integral equation approach[2] to studying first passage time problems of diffusion processes in an oscillating field. If the diffusion problem has symmetry around the origin, then $W_1(t) = 0$ and $G_0^-(t, t') = 0$ and Eq. (13) for $k = 0$ alone needs to be considered. Such a case, with application to delayed bifurcation in a noisy dynamical system, was studied earlier.[4] For the present situation, we assume that the particle starts at $x = 0$ at $t = 0$ so that $P_{\text{in}}(x) = \delta(x)$. Then, $P_\infty(x, t) = G(x, t \mid 0, 0)$ and the source functions of Eq. (14) can be obtained by integrating over x in $[-1, 1]$. The results expressed in terms of Gaussian integrals are

$$\begin{aligned} S_0(t) &= \frac{1}{\sqrt{\pi}} \int_{z_-}^{z_+} \exp(-q^2) \, dq \equiv F(z_-, z_+) \\ S_1(t) &= \left\{ \frac{t}{\pi} \right\}^{1/2} [\exp(-z_-^2) - \exp(-z_+^2)] + V(t, 0) \, S_0(t) \end{aligned} \tag{16}$$

with

$$z_\pm(t) = \frac{\pm 1 - V(t, 0)}{2\sqrt{t}} \tag{17}$$

The function $F(z_-, z_+)$ can be expressed in terms of error functions. In a similar manner, the kernel functions of Eq. (15) can be written as

$$G_0^{\pm}(t, t') = \frac{1}{2} [F(a_-, a_+) \pm F(b_-, b_+)] \tag{18}$$

$$\begin{aligned} G_1^{\pm}(t, t') = \left\{ \frac{t - t'}{4\pi} \right\}^{-1/2} &\{ [\exp(-a_-^2) - \exp(-a_+^2)] \\ &\pm [\exp(-b_-^2) - \exp(-b_+^2)] \} \\ &+ G_0^+(t, t') \frac{V(t, t') + 1}{2} \pm G_0^-(t, t') \frac{V(t, t') - 1}{2} \end{aligned} \tag{19}$$

with

$$a_\pm(t) = \frac{\pm 1 - 1 - V(t, t')}{2(t - t')^{1/2}}, \qquad b_\pm(t) = \frac{\pm 1 + 1 - V(t, t')}{2(t - t')^{1/2}} \tag{20}$$

To compute numerically the solution of the integral equations (13) for $W_k(t)$, we divide the time axis into intervals, the nth interval being of length $\delta_n = t_n - t_{n-1}$. We assume that δ_n $(n \geqslant 1)$ are small and hence $W_k(t)$ can be approximated by a linear function in each interval. That is, for $t_{n-1} \leqslant t \leqslant t_n$,

$$W_k(t) = \frac{1}{\delta_n} [W_k(t_{n-1})(t_n - t) + W_k(t_n)(t - t_{n-1})] \tag{21}$$

Then $W_k(n) \equiv W_k(t_n)$ can be expressed as

$$\begin{aligned} W_k(n) = S_k(n) &+ \sum_{m=1}^{n} B_k^+(n, m)[W_0(m) - W_0(m-1)] \\ &+ \sum_{m=1}^{n} B_k^-(n, m)[W_1(m) - W_1(m-1)] \\ &- \sum_{m=1}^{n} [C_k(n, m)\, W_0(m) + D_k(n, m)\, W_0(m-1)], \qquad n \geqslant 0 \end{aligned} \tag{22}$$

The matrix elements in Eq. (22) are defined as

$$\begin{aligned} B_k^{\pm}(n, m) &= \frac{1}{\delta_m} \int_{t_{m-1}}^{t_m} G_k^{\pm}(t_n, t')\, dt' \\ C_k(n, m) &= \frac{1}{\delta_m} \int_{t_{m-1}}^{t_m} G_k^{-}(t_n, t')\, v(t')(t' - t_{m-1})\, dt' \\ D_k(n, m) &= \frac{1}{\delta_m} \int_{t_{m-1}}^{t_m} G_k^{-}(t_n, t')\, v(t')(t_m - t')\, dt' \end{aligned} \tag{23}$$

Following our earlier work,[4] we approximate the integrals in Eq. (23) using a three-point Simpson's rule to get

$$\begin{aligned} B_k^{\pm}(n, m) &= \tfrac{1}{6}[G_k^{\pm}(t_n, t_m) + 4G_k^{\pm}(t_n, t_m - \delta_m/2) + G_k^{\pm}(t_n, t_{m-1})] \\ C_k(n, m) &= \tfrac{1}{6}\delta_m[G_k^{-}(t_n, t_m)\, v(t_m) + 2G_k^{-}(t_n, t_m - \delta_m/2)\, v(t_m - \delta_m/2)] \\ D_k(n, m) &= \tfrac{1}{6}\delta_m[2G_k^{-}(t_n, t_m - \delta_m/2)\, v(t_m - \delta_m/2) + G_k^{-}(t_n, t_{m-1})\, v(t_{m-1})] \end{aligned} \tag{24}$$

Now, the simultaneous recurrence relations of Eq. (22) can be solved at each time point t_n $(n \geqslant 0)$ until $W_k(n)$ becomes negligibly small for n sufficiently large, say $n \geqslant N$. All the moments of the first passage time distribution can then be calculated. For instance, the mean first passage time is given by

$$\tau \equiv \int_0^t W_0(t)\, dt = \frac{1}{2} \sum_{m=1}^{N} [W_0(m) + W_0(m-1)] \tag{25}$$

Results for first passage time distributions to be discussed below were computed using the approximation

$$g(t_m - \delta_m/2) = (1/\delta_m)[W_0(m) - W_0(m-1)] \tag{26}$$

In view of the oscillating nature of $W_k(t)$ and $g(t)$, to be expected at higher frequencies, it is necessary to use sufficiently small time steps $\{\delta_m\}$ in the above formulas. We have employed an automatic time step generation technique well developed in numerical approximations to solutions of differential equations.[5] The term neglected in the linear approximation of $W_0(t)$ over the nth interval is bounded by $|W_0''(n-1)|\,\delta_n^2/2$, where $W_0''(n-1)$ denotes the second derivative of W_0 at t_{n-1}. We determine δ_n with the condition[5]

$$\frac{1}{2W_0(n)}\,|W_0''(n-1)|\,\delta_n^2 \leqslant E_r \tag{27}$$

where E_r is some specified error criterion, say, 10^{-3}. The error term in the Simpson's rule leading to Eqs. (24) is $O(\delta_n^5)$ and hence may be ignored in estimating δ_n. To determine δ_n from Eq. (27), we use the three-point difference formula [employing $W_0(n)$, $W_0(n-1)$, and $W_0(n-2)$] to estimate $W_0''(n-1)$, and we employ the following marching scheme through the time intervals starting at $n=0$. After obtaining the initial values $W_k(0)$

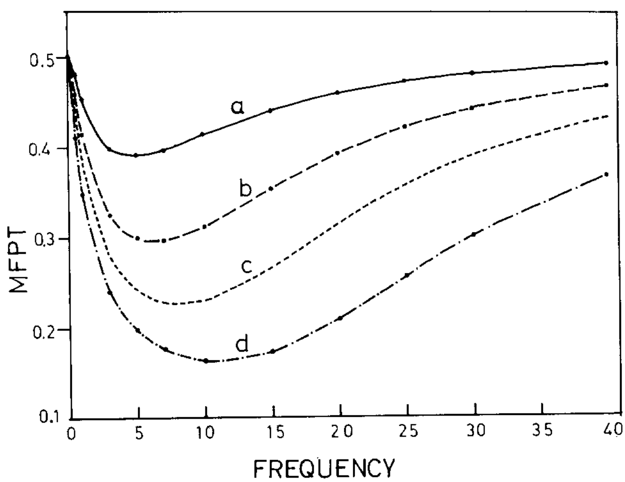

Fig. 1. Mean first passage time (MFPT) vs. frequency ω for (a) $\varepsilon=3$, (b) $\varepsilon=5$, (c) $\varepsilon=7$, (d) $\varepsilon=10$.

from $S_k(0)$, we calculate $W_k(1)$ with a sufficiently small input value δ_1, say, 10^{-3}. Next, $W_k(2)$ is computed with a starting guess value $\delta_2 = \delta_1$ and the l.h.s. of Eq. (27) is estimated for $n = 2$. If the criterion is satisfied, then calculation proceeds to the next step, that is, $n = 3$. Otherwise, δ_2 is picked using Eq. (27) (with the equality sign) and $W_k(2)$ is recalculated. This procedure is repeated until the error criterion is satisfied. Calculations then proceed to the next time step.

The ω dependence of the mean first passage time $\tau(\omega)$ calculated using this procedure for values of $\varepsilon = 3, 5, 7$, and 10 is shown in Fig. 1. $\tau(\omega)$ initially deceases from its unbiased value $\tau(0) = 0.5$[1] (in reduced units) at $\omega = 0$, attains a minimum (depending on the magnitude of ε), and then increases as ω becomes larger. This behavior may be understood as follows. There are two time scales in the process, namely $\tau(0)$, which may be called the "diffusion time," and the half period π/ω of $v(t)$ during which the field acts along one direction. For values of ω such that $\tau(0) \leqslant \pi/\omega$, the field guides the particle out of the domain $[-1, 1]$ within the diffusion time. Thus, one would expect $\tau(\omega)$ to decrease at smaller ω. At larger ω, when π/ω becomes smaller compared to $\tau(0)$, the field forces the particle to move to the right and left about the origin, the strength of the force being dependent on ε. Then, exit of trajectories from the domain $[-1, 1]$ is mainly controlled by diffusion and thus an increase in mean first passage time is expected. In the limit when $\pi/\omega \ll \tau(0)$, the field would have a negli-

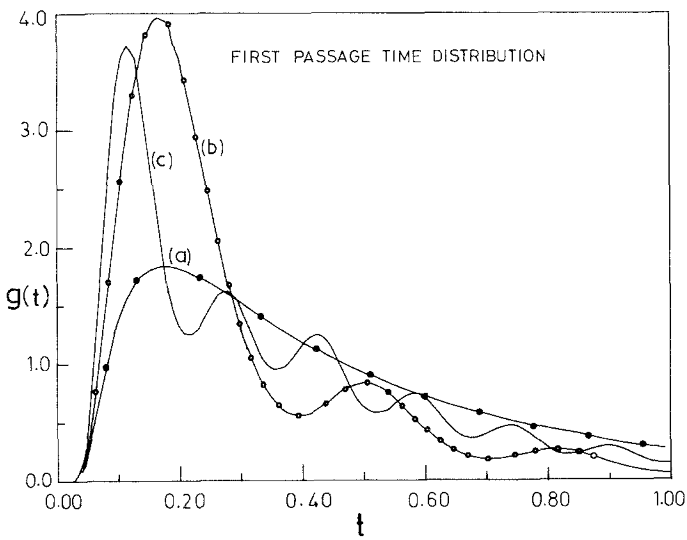

Fig. 2. First passage time distribution $g(t)$ vs time t for $\varepsilon = 5$ and (a) $\omega = 0$, (b) $\omega = 5$, (c) $\omega = 10$.

gible effect on the particle and $\tau(\omega)$ approaches $\tau(0)$. These observations agree qualitatively with the simulation data.[1] The method of treating the drift field as a perturbation[1,6] will be completely inadequate for the range of ε necessary to show the full frequency dependence of mean first passage time.

The first passage time distribution $g(t)$ for $\varepsilon = 5$ and $\omega = 0$, 5, and 10 is shown in Fig. 2. The rather fast initial rise in $g(t)$ for $\omega = 5$ (say), in comparison to the case of $\omega = 0$, is due to the exit of trajectories in the first half cycle of $v(t)$. The subsequent fall in $g(t)$ is triggered by the reversal of $v(t)$, which inhibits the escape of trajectories. For later times, $g(t)$ has a damped oscillatory nature characteristic of ω. These oscillations result from the particle motion around the origin induced by the field. As ω increases, the first peak in $g(t)$ occurs earlier and oscillations are centered about the zero-frequency curve.

The dependence of the mean first passage time on other parameters[1] of the problem, such as different initial distributions, phase of the drift field, etc., can be easily studied using the present method. Note that we have shown that it is unnecessary to solve numerically the complete Fokker–Planck equation[1] in the bounded domain for studying first passage time problems in time-dependent fields.

Finally, we remark that there is a large literature[7] employing Siegert's integral equation theory for a related class of first passage time problems of diffusion processes in the presence of time-dependent boundaries. Numerical as well as analytical studies on first passage time densities have been reported.

ACKNOWLEDGMENTS

I thank the referees for pointing out the related work in ref. 7 and for suggestions for improving the presentation of this paper.

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Communicated by J. L. Lebowitz