First-passage-time distribution for diffusion through a planar wedge

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We obtain compact, exact, analytical expressions for the first-passage-time distribution for a particle diffusing on a planar wedge for special values of the wedge angle. Specifically, we calculate the first-passage-time distribution for the diffusing particle through a planar wedge of angle π/n, where n is an integer. For the cases $n=2$ and n odd, we provide an exact closed-form expression to the first-passage-time distribution while for the remaining cases, we provide it in integral form and evaluate numerically using quadratures. We then show that our results are in good agreement with Markovian simulations in the continuum limit.

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I. INTRODUCTION

The first-passage-time distribution (FPTD) is a probabilistic measure associated with the time required for a stochastic process to reach some specified values [1]. It has been applied in the study of biological processes [2–4]. Polymer translocation [5–9], and transient dynamics of laser [10–12]. While the study of FPTD has its many applications, there are only a limited number of exactly solvable models found in the literature. Among those solved in the literature are in one-dimension [1], in a half-plane [13], and in a planar wedge with interior angle $\pi/3$ [14,15].

The FPTD through a planar wedge has been studied previously in [1,13] for arbitrary wedge angles. However, the FPTD expressions obtained were valid only in the asymptotic long time limit. The difficulty in obtaining closed-form expressions stems from the unwieldy series expressions that result from the solution to the diffusion equation for arbitrary planar angles. In this paper we show that exact, compact, analytical expressions for the FPTD can be obtained provided that the analysis is restricted to special values of the wedge angle. Specifically, we investigate the properties of diffusion through a planar wedge with wedge angle π/n where n is a positive integer. To obtain exact solutions, we limit the wedge angles to π/n, where n is an integer. We will then show that for several cases of n, we can obtain exact-closed form expressions for FPTD and for the rest of the cases, the problem reduces to an integral that can be evaluated numerically. We will also show that our results are in good agreement with Markovian simulations in the continuum limit.

II. PROBABILITY DENSITY FUNCTION

The first task in finding the FPTD is finding the probability density function (PDF) of an equivalent system with absorbing planar wedge boundaries. We consider an isotropic diffusing particle initially at (x_0,y_0) constrained in a wedge of angle π/n, where n is a positive integer, and with absorbing planar wedge boundaries as shown in Fig. 1. The PDF is therefore the solution to the isotropic diffusion equation

$$D\nabla^2\rho(x,y;t)=\frac{\partial}{\partial t}\rho(x,y;t). \tag{1}$$

with initial condition $\rho(x,y;0)=\delta(x-x_0)\delta(y-y_0)$. The absorbing boundary condition requires our solution to have the following conditions:

$$\lim_{x=0}\rho(x,y;t)=\lim_{y=x\tan\gamma}\rho(x,y;t)=0, \tag{2}$$

where for convenience, we define $\gamma\equiv\pi/n$ as the angle of the planar wedge.

To solve this partial differential equation, we recall the Green's function for the unbounded diffusion equation as

$$G(x,y;t)=\frac{1}{4\pi Dt}e^{-[(x-x_0)^2+(y-y_0)^2]/4Dt}. \tag{3}$$

In the presence of the absorbing boundaries, the solution is just a superposition of the Green's function of sources and sinks distributed uniquely throughout the plane. In Fig. 1, the dark-colored dot represents one of the sources and the light-colored dot represents one of the sinks. We wish to find the position of the sink in this figure, which is just the mirror image of the source. With a bit of geometry, we see that the position of the sink is at (x_0^-,y_0^-), where

$$x_0^-=r_0\cos(2\gamma-\alpha),$$
$$y_0^-=r_0\sin(2\gamma-\alpha). \tag{4}$$

Here, $r_0=\sqrt{(x_0)^2+(y_0)^2}$ and $\alpha=\mathrm{Arctan}(y_0/x_0)$ are the polar components. To find the distribution of the sources (and sinks), we note that they lie on a circle of radius r_0 and spaced at an angle 2γ apart. The sources are therefore at

$$x_k^+=r_0\cos(\alpha+2k\gamma),$$

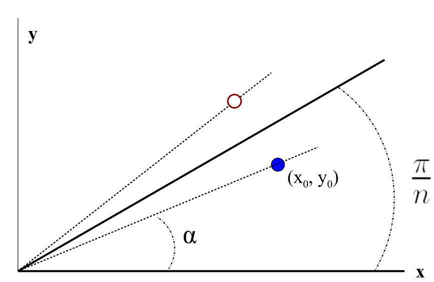

FIG. 1. (Color online) Geometry of the wedge problem. The dark-colored dot represents the diffusing particle's initial position and light-colored dot is one of its images.

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$$y_k^+ = r_0 \sin(\alpha + 2k\gamma), \quad k = 0,1, \ldots ,n-1, \tag{5}$$

and the sinks are at

$$x_k^- = r_0 \cos[(2+2k)\gamma - \alpha],$$
$$y_k^- = r_0 \sin[(2+2k)\gamma - \alpha], \quad k = 0,1, \ldots ,n-1. \tag{6}$$

We can now write our PDF for this system as

$$\rho(x,y;t)_{x,y\in\mathcal{R}} = \frac{1}{4\pi D t}\sum_{k=0}^{n-1} e^{-[(\bar{x}-\bar{x}_k^+)^2+(\bar{y}-\bar{y}_k^+)^2]/t} - e^{-[(\bar{x}-\bar{x}_k^-)^2+(\bar{y}-\bar{y}_k^-)^2]/t}, \tag{7}$$

where the barred coordinates are scaled such that $\bar{z}=z/\sqrt{4D}$. In the region outside the planar wedge, the PDF vanishes. It is straightforward to show that the PDF vanishes at the boundaries, $y=0$ and $y=x \tan \gamma$.

III. SURVIVAL PROBABILITY

The presence of the absorbing boundaries causes the survival probability, $S(t)$ to monotonically decrease in time. We can solve this by integrating the PDF over all space, i.e.,

$$S(t) = \int_0^{+\infty} dx \int_0^{x \tan \gamma} dy \rho(x,y;t). \tag{8}$$

Evaluation of this integral to a closed-form expression is not trivial. In this Brief Report, we provide a closed-form expression for the cases where n is odd and $n=2$. For the remaining cases, we provided it in integral form as well as an infinite series. We shall treat each case separately in the next sections.

A. Survival probability when n is odd

The evaluation of the integral (8) can be solved exactly and in closed form when n is odd by exploiting symmetries of the distribution of the sources and sinks, and that of the PDF itself. We first consider the case where the particle is initially at $(r_0 \cos \frac{\gamma}{2}, r_0 \sin \frac{\gamma}{2})$, or when the particle is on the symmetry axis of the wedge. From the expressions in (5) and (6), we see that the sources and sinks are in opposite locations with respect to the origin. We can see that the PDF for this case is an odd function about the origin. Evaluating the integral $\int_0^{x \tan \gamma} \rho(x,y;t) dy$ leads to an even function in x. To perform the remaining integration, we use the identity

$$\int_{-\infty}^{\infty} e^{-(\alpha x+\beta)^2} \operatorname{erf}(\gamma x+\delta) dx = \frac{\sqrt{\pi}}{\alpha} \operatorname{erf}\left(\frac{\alpha\delta-\beta\gamma}{\sqrt{\alpha^2+\gamma^2}}\right). \tag{9}$$

When the particle is not initially on the symmetry axis, the source or sink are no longer in opposite locations. However, we use the following trick of introducing an auxiliary particle at $[r_0 \cos(\gamma-\alpha), r_0 \sin(\gamma-\alpha)]$. For the specific case $n=3$, the positions for the particles and its respective images are shown in Fig. 2. The survival probability of the original and auxiliary particle are identical. With the addition of the auxiliary particle, the source and sink pairs are again at opposite locations with respect to the origin. With this, we finally get the result

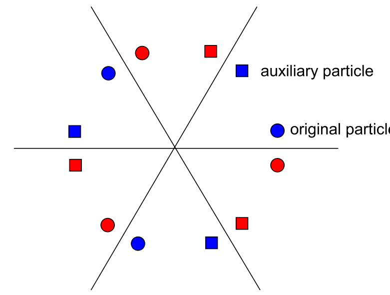

FIG. 2. (Color online) Positions of the sources and sinks of the original and auxiliary particle for the specific case $n=3$.

$$S(t) = \sum_{k=0}^{n-1} \frac{(-1)^k}{4}\left[\operatorname{erf}\left(\frac{\bar{r}_0 \sin(k\gamma+\alpha)}{\sqrt{t}}\right) + \operatorname{erf}\left(\frac{\bar{r}_0 \sin(\alpha-k\gamma)}{\sqrt{t}}\right) + \operatorname{erf}\left(\frac{\bar{r}_0 \sin[(k+1)\gamma-\alpha]}{\sqrt{t}}\right) + \operatorname{erf}\left(\frac{\bar{r}_0 \sin[(1-k)\gamma-\alpha]}{\sqrt{t}}\right)\right]. \tag{10}$$

The long time limit for this distribution gives the first-order contribution

$$\lim_{t\to\infty} S(t) = \left(\frac{\bar{r}_0}{\sqrt{t}}\right)^n \sum_{k=0}^{n-1} (-1)^{k+(n-1)/2}\left(\frac{\sin^n(k\gamma+\alpha)}{2n(n-1)} + \frac{\sin^n(\alpha-k\gamma)}{2n(n-1)} + \frac{\sin^n[(k+1)\gamma-\alpha]}{2n(n-1)} + \frac{\sin^n[(1-k)\gamma-\alpha]}{2n(n-1)}\right). \tag{11}$$

This result is consistent with the result in [1], i.e., $\lim_{t\to\infty} S(t) \propto (r_0/\sqrt{t})^n$. As a specific case, let us consider the diffusion of a particle in a half-plane and initially at (x_0,y_0) where $x_0,y_0>0$. For a half-plane $(n=1)$, the survival probability is

$$S(t)_{(n=1)} = \operatorname{erf}\left(\frac{\bar{r}_0 \sin \alpha}{\sqrt{t}}\right) = \operatorname{erf}\left(\frac{\bar{y}_0}{\sqrt{t}}\right), \tag{12}$$

which is expected [13]. For the wedge of angle $\frac{\pi}{3}$, we obtain:

$$S(t)_{(n=3)} = \operatorname{erf}\left(\frac{\bar{y}_0}{\sqrt{t}}\right) + \operatorname{erf}\left(\frac{\sqrt{3}\bar{x}_0-\bar{y}_0}{2\sqrt{t}}\right) - \operatorname{erf}\left(\frac{\sqrt{3}\bar{x}_0+\bar{y}_0}{2\sqrt{t}}\right). \tag{13}$$

Computation of $S(t)$ for other n is straightforward.

B. Survival probability when n is even

We next tackle $S(t)$ for the absorbing wedge of angle π/n, where n is an even integer. We can take the series solution for the integral (8),

$$S(t) = \sum_{k=0}^{(n/2)-1} \operatorname{erf}\left(\frac{\bar{x}_0}{\sqrt{t}}\right)\operatorname{erf}\left(\frac{\bar{y}_0}{\sqrt{t}}\right) + \lim_{\beta=1} \sum_{k=0}^{(n/2)-1} \sum_{m=0}^{\infty} \frac{(2\bar{x}_k)^{(2m+1)}}{(2m+1)!} \frac{d^m}{d\beta^m} e^{-(x_k^2+\bar{y}_k^2 \cos^2 \gamma)/t} \times \frac{\sin \gamma}{\sqrt{t+t\beta}}\left\{e^{-\bar{y}_k^2 \sin^2 \gamma/(t+t\beta)}\left[1+\operatorname{erf}\left(\frac{\bar{y}_k \sin \gamma}{\sqrt{t+t\beta}}\right)\right]\right\}. \tag{14}$$

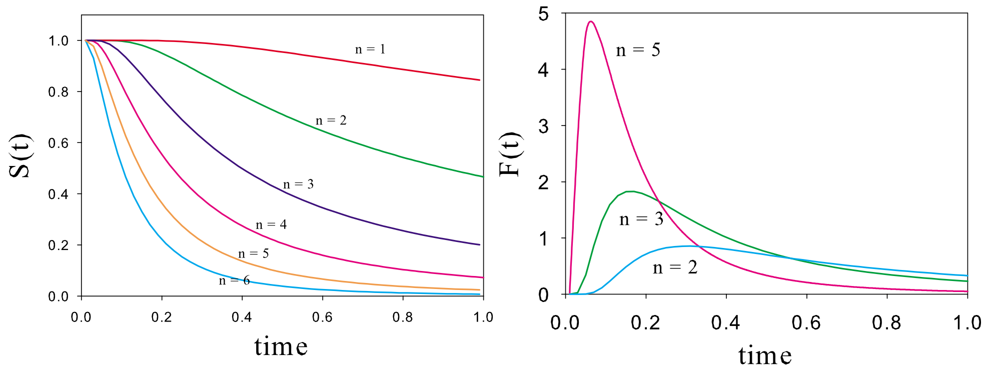

FIG. 3. (Color online) Survival probability and first-passage-time distribution for diffusing particle initially at $(2\cos\frac{\pi}{2n}, 2\sin\frac{\pi}{2n})$ and $D=1$ for various n. For the case $n \in \{1,2,3,5\}$, $S(t)$ comes from an exact expression. For $n=4,6$, $S(t)$ was computed numerically.

For the case $n=2$, the sum can be evaluated to

$$S(t)_{(n=2)} = \operatorname{erf}\left(\frac{\bar{x}_0}{\sqrt{t}}\right)\operatorname{erf}\left(\frac{\bar{y}_0}{\sqrt{t}}\right). \qquad (15)$$

For the remaining cases ($n \neq 2$), we have not found an exact, closed-form expression of this sum, but we can evaluate the integral numerically. In this work, we use Clenshaw-Curtis integration quadrature. We refer the reader to [16] for more information about this method. We numerically evaluated the integral in the interval $t=[0,13]$. For the case $n=4$, evaluation was done at 100 equidistant times. For the case $n=6$, we reduce this number to 50 points as evaluations require a more powerful machine. The maximum error tolerance was set to 10 decimal places. The survival probability is plotted in Fig. 3.

In evaluating $S(t)$ for the even n case, we can see the advantage of having an exact expression in the odd n case as the former requires high computing power and longer evaluation times. The reason is that the number of terms in these integrals increases exponentially as n increases. However, for the exact expression for the odd n case, (10) requires only evaluation of n terms at prescribed times. An important extension for this work is to find an exact expression for the even n case.

IV. FIRST-PASSAGE-TIME DISTRIBUTION

The first-passage-time distribution, $F(t)$ can be computed from the relation

$$F(t) = -\frac{d}{dt}S(t). \qquad (16)$$

Since we have an exact expression when n is odd, then we can provide the exact $F(t)$ for this case as

$$\begin{aligned} F(t) = \sum_{k=0}^{n-1} \frac{(-1)^k \bar{r}_0}{\sqrt{\pi} t^{3/2}} \Bigg(& \frac{\sin[(1-k)\gamma-\alpha]}{4} e^{-\bar{r}_0^2 \sin^2[(1-k)\gamma-\alpha]/t} \\ & + \frac{\sin(\alpha-k\gamma)}{4} e^{-\bar{r}_0^2 \sin^2(\alpha-k\gamma)/t} \\ & + \frac{\sin(k\gamma+\alpha)}{4} e^{-\bar{r}_0^2 \sin^2(k\gamma+\alpha)/t} \\ & + \frac{\sin[(k+1)\gamma-\alpha]}{4} e^{-\bar{r}_0^2 \sin^2[(k+1)\gamma-\alpha]/t} \Bigg). \end{aligned} \qquad (17)$$

The long time limit for this expression is

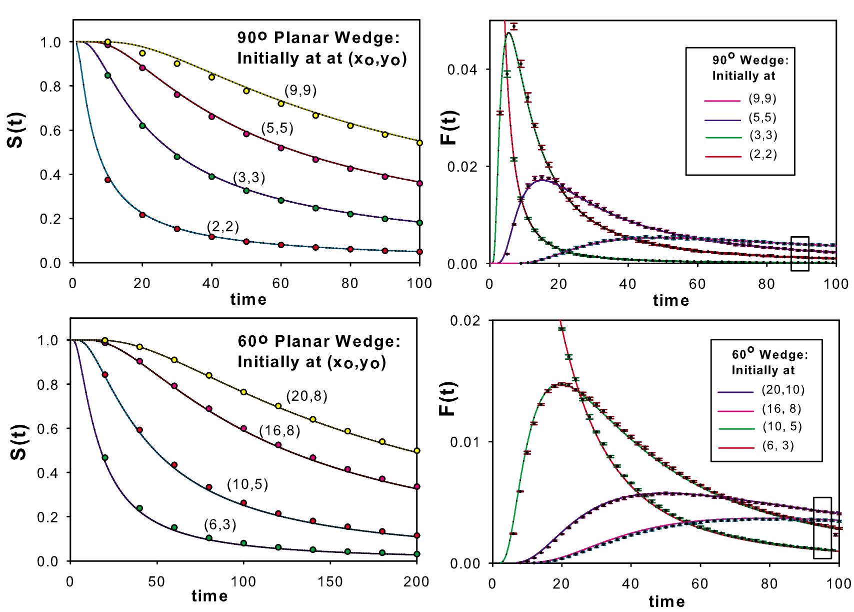

FIG. 4. (Color online) Survival probability and first-passage-time distribution for 1-million walkers initially at (x_0, y_0). Solid line refers to the diffusion prediction and the markers are simulation points. The standard deviation is computed over 10 simulation runs.

$$\lim_{t\to\infty} F(t) = \frac{n}{2t} \lim_{t\to\infty} S(t). \tag{18}$$

This result is consistent with the result in [1], i.e. $\lim_{t\to\infty} F(t) \propto t^{-[(n/2)+1]}$. We give explicitly the expressions for several cases of n. For the half-plane geometry ($n=1$), we have the following FPTD:

$$F(t)_{(n=1)} = \frac{\bar{r}_0 \sin\alpha}{\sqrt{\pi} t^{3/2}} e^{-\bar{r}_0^2 \sin^2 \alpha/t} = \frac{\bar{y}_0}{\sqrt{\pi} t^{3/2}} e^{-\bar{y}_0^2/t}, \tag{19}$$

which is expected [13]. For the case $n=3$, the FPTD is

$$F(t)_{(n=3)} = \frac{\bar{y}_0}{\sqrt{\pi} t^{3/2}} e^{-\bar{y}_0^2/t} + \frac{\bar{r}_0 \cos\left(\alpha + \dfrac{\pi}{6}\right)}{\sqrt{\pi} t^{3/2}} e^{-\bar{r}_0^2 \cos^2[\alpha+(\pi/6)]/t} - \frac{\bar{r}_0 \sin\left(\alpha + \dfrac{\pi}{3}\right)}{\sqrt{\pi} t^{3/2}} e^{-\bar{r}_0^2 \sin^2[\alpha+(\pi/3)]/t}, \tag{20}$$

which is equivalent to an earlier result by O'Connell and Unwin [15]. Taking the average of the above equation over all angles from 0 to $\pi/3$ and setting $r_0=1$ leads to Eq. (31) of Comtet and Desibois [14]. Computations of FPTD for other odd values of n is straightforward.

When n is even, we can provide an exact closed-form expression for the quarter-plane case ($n=2$) since we can solve $S(t)$ exactly in (15),

$$F(t)_{(n=2)} = \frac{\bar{x}_0}{\sqrt{\pi} t^{3/2}} \operatorname{erf}\left(\frac{\bar{y}_0}{\sqrt{2t}}\right) e^{-\bar{x}_0^2/t} + \frac{\bar{y}_0}{\sqrt{\pi} t^{3/2}} \operatorname{erf}\left(\frac{\bar{x}_0}{\sqrt{2t}}\right) e^{-\bar{y}_0^2/t}. \tag{21}$$

For the remaining cases, we can differentiate the expression in (14) to obtain a series expression. We can also numerically integrate using quadratures. We plot the FPTD for different parameter values in Fig. 3.

V. MARKOVIAN SIMULATION

The Markovian process can be approximated by the diffusion equation in the continuum limit. Here, we consider the unbiased two-dimensional (2D) random walk in a square lattice of spacing s. The probability of the particle at the $(n+1)$th step to be on (x,y), $P_{n+1}(x,y)$, can be expressed as

$$P_{n+1}(x,y) = \tfrac{1}{4}P_n(x+s,y) + \tfrac{1}{4}P_n(x-s,y) + \tfrac{1}{4}P_n(x,y+s) + \tfrac{1}{4}P_n(x,y-s). \tag{22}$$

This difference equation governs the evolution of the particle for all time steps and positions given some initial conditions. The discreteness of this formulation makes this amenable to numerical simulations. Through Taylor series expansion of (22) about the point (x,y), and taking the continuum limit, we obtain the diffusion equation

$$\frac{\partial}{\partial n}\mathcal{P}(x,y) = D\nabla^2\mathcal{P}(x,y), \tag{23}$$

where $D \equiv \frac{s^2}{4\Delta n}$. Here $\mathcal{P}(x,y)$ is the continuum limit probability distribution function and $\nabla \equiv \partial_x^2 + \partial_y^2$. This means that the unbiased 2D random walk can be explained by the diffusion equation in the continuum limit. This result will be used for comparison with the analytical results derived from the study of the diffusion equation.

We simulate a random walk of a particle initially for the quarter plane and for 60° planar wedge. To simulate the effect of absorbing boundaries, we set the condition that if the particle reaches the boundary, it will stay on the boundary for all time steps, and will be treated as if it has died. We iterate this procedure for a sufficient number of particles, each evolved one at a time to satisfy the noninteracting condition. We use the random number generator MT19937 (Mersenne Twister) [17]. Our measurements in these simulations are the number of surviving particles, or the number of iterated particles that are not on the boundary at time step t. Also, we measure the time it takes for each particle to reach the boundary, thus creating an absorbing time distribution. The results are shown in Fig. 4.

From the results, it can be seen that the prediction of the diffusion equation is in good agreement with the restricted Markovian simulation in the continuum limit. The relative difference for short times can be accounted for by the continuum limit approximation. This result is very useful as the numerical computations from the diffusion prediction are by far faster than Markovian simulations for a large number of iterations.

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