Arch. Rational Mech. Anal. 203 (2012) 329–342
Digital Object Identifier (DOI) 10.1007/s00205-011-0455-6

Analytical and Numerical Results for an Escape Problem

Carey Caginalp & Xinfu Chen

Communicated by C. Dafermos

Abstract

A particle moves with Brownian motion in a unit disc with reflection from the boundaries except for a portion (called a "window" or "gate") in which it is absorbed. The main problems are to determine the first hitting time and spatial distribution. A closed formula for the mean first hitting time is discovered and proven for a gate of any size. Also given is the probability density of the location where a particle hits if initially the particle is at the center or uniformly distributed. Numerical simulations of the stochastic process with finite step size and a sufficient number of sample paths are compared with the exact solution to the Brownian motion (the limit of zero step size), providing an empirical formula for the difference. Histograms of first hitting times are also generated.

1. Introduction

Many physical, chemical, biological and ecological processes can be formulated in terms of Brownian motion with reflection at most of the domain boundary and absorption from a small part. In chemical processes [10], particle A may move around randomly while B is essentially stationary, and a reaction occurs when A enters an attraction basin of B. In cell biology, an ion drifts about within a cell, is reflected when it hits the membrane, which is most of the boundary of the cell, and escapes when it hits a small pore, thereby altering the electrostatic balance in and out of the cell [4]. A prey moving randomly in a confined territory dies when it encounters a predator hiding at the entrance to the territory [7]. An epidemic confined in one region may spread through a small unsecured boundary of the region.

These applications thus lead to a pure mathematical problem of finding the expected lifetime (mean first passage time or MFPT) of a Brownian particle in an n-dimensional domain Ω in which the particle is reflected from $\partial\Omega\setminus\Gamma$ and dies (or escapes or is absorbed) once it hits $\Gamma \subseteq \partial\Omega$. This problem has been studied by several authors ([2,3,5–7,9] and references therein). Most recently, CHEN and FRIEDMAN [1] proved asymptotic expansions for MFPT when the size of the gate, Γ, is small.

In this paper, we present and prove a closed formula for MFPT for the fundamental case when Ω is the unit disc and Γ is a connected arc on the boundary. From an analytical point of view this formula provides the exact size of $O(1)$ coefficient in several asymptotic expansions derived in the past [1,2,4,5,9]. We call the case fundamental since based upon it, asymptotic expansions for general domains with multiple small windows can be derived [1]. From a numerical point of view, this formula provides a reliable test for any numerical algorithm designed to tackle the case when the gate size is very small (so the numerical problem is very stiff). In general, without knowing the exact size of $O(1)|\Gamma|$ or even $O(1)|\Gamma|^2$, where $|\Gamma|$ is the length of Γ, an asymptotic expansion is quite often very hard to verify or use, since one cannot easily determine whether the difference between the numerical solution and the asymptotic expansion is due to the error of discretization or due to the error, say, $O(1)|\Gamma|\log|\Gamma|$, of the underlying asymptotic expansion. Our closed formula provides a concrete criterion here.

As a consequence of the relationship between the stochastic problem and elliptic equations (see Theorem 1) one can compute numerical solutions on MFPT using Poisson's equation. Here we shall use a Monte–Carlo method directly simulating the diffusion process and computing related statistics. A simple Monte–Carlo simulation can produce a tremendous amount of useful information. For example, from a reasonable amount ($\geqq 20$) of sample paths, we can construct a histogram of exit times (Fig. 1) from which we can compute the mean (that is MPFT), the variance, the probability density (and its exponential tail), etc., of the first passage times; also, from the locations of exits, we can construct histograms as well as empirical cumulative distribution functions (Fig. 4) to find where the particle exits. A single 2 GHz processor can produce 10^6 sample paths per hour if the time step, Δt, and the size of the gate are not too small, say $\Delta t \geqq 10^{-5}$ and $|\Gamma| \geqq 10^{-1}$. In applications, this will be sufficient to provide needed information for actions of optimal controls.

Our Monte–Carlo simulation is based on the following stochastic process, $\{X_t, Y_t\}_{t\in\mathbf{T}}$, defined by

$$Y_{t+\Delta t} = X_t + \sqrt{\Delta t}\,\eta_t, \qquad X_{t+\Delta t} = \frac{Y_{t+\Delta t}}{\max\{1, |Y_{t+\Delta t}|^2\}} \quad \forall\, t \in \mathbf{T} := \bigcup_{k=0}^{\infty}\{k\Delta t\}, \tag{1}$$

where $X_0 = Y_0$ are given and $\{\eta_t\}_{t\in\mathbf{T}}$ are independent and identically distributed random variables with (normal) $N(\mathbf{0}, \mathbf{I})$ distribution. The first passage time associated with the process is defined by

$$\tau^* = \min\left\{t \in \mathbf{T} \;\middle|\; \frac{Y_t}{\max\{1, |Y_t|\}} \in \Gamma\right\}. \tag{2}$$

In simulation, first of all, there is a random error due to the statistical sampling. Trusting the quality of the common random number (CRN) generator that we use,

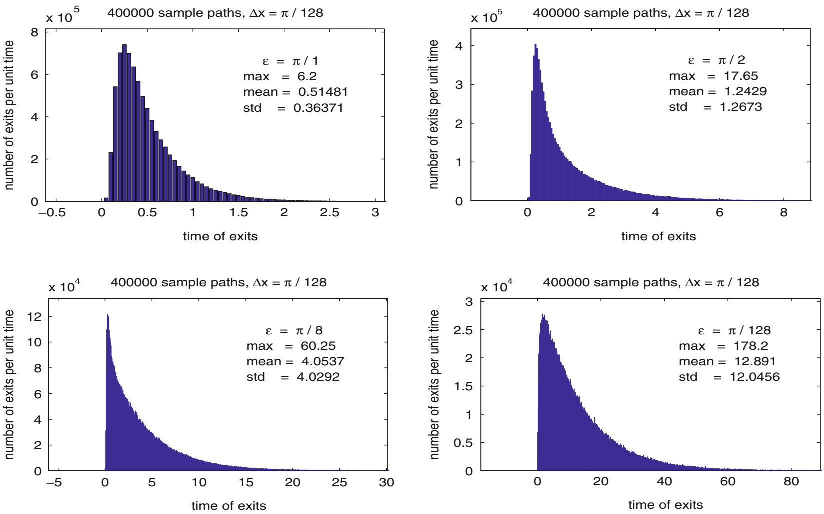

Fig. 1. The histograms of exit times, where max represents the longest time of exit among all sample paths

this error can be controlled by taking an appropriately large number of samples, as a consequence of the Central Limit Theorem. There is also a discretization error due to the approximation of (1) to the diffusion process, $\{W_t\}_{t\geq 0}$, of the Brownian motion confined in the unit disc with pure reflection on the boundary. With an exact solution for the particular case of the circle, one can then obtain empirical results as step size and gate size vary. Thus, a careful comparison of the exact solution with the numerical solution illuminates the distinction between finite steps and continuous diffusion.

Note that replacing the $N(\mathbf{0}, \mathbf{I})$ distribution of η_t by a certain transition distribution that depends on X_t will diminish the discretization error. We hope that one can either find a convenient way to use the transition density from W_t to $W_{t+\Delta t}$ to eliminate the discretization error or find the asymptotic behavior, as $\Delta t \to 0$, of the distribution difference between $\{X_t\}_{t\in\mathbf{T}}$ and $\{W_t\}_{t\geq 0}$. We also hope to find the distribution difference between the stopping time τ^* defined in (2) and the first passage time $\tau := \inf\{t > 0 \mid W_t \in \Gamma\}$ in order to produce a correction for the discretization error. Our simulation with $X_0 = (0, 0) = W_0$ suggests that

$$\frac{1}{2} - 2\log\left(\sin\frac{|\Gamma|}{4}\right) = \mathbb{E}[\tau] \approx \mathbb{E}[\tau^*] - \frac{4\sqrt{\Delta t}}{|\Gamma|}, \qquad \text{std}[\tau^*] \approx \mathbb{E}[\tau^*], \tag{3}$$

where $\mathbb{E}$ stands for expectation and std the standard deviation; see Figs. 1 and 3 where $\varepsilon = |\Gamma|/2$, $\Delta x = \sqrt{\Delta t}$, and MCT is the sample mean $\approx \mathbb{E}[\tau^*] + N(0, \text{std}[\tau^*]^2/n)$ with $n = 400{,}000$.

The rest of the paper is organized as follows. We present our theoretical results for $\mathbb{E}[\tau]$ and $\text{std}[\tau]$ in Section 2, their proofs in Section 3, and results of Monte–Carlo simulations in Section 4. An announcement of the results has appeared in C.R. Math Acad. Sci. Paris 349 (2011) 191–194.

2. Main Results

Our starting point is the formulation for the statistics of the stochastic process as solutions of differential equations. The following equation for the mean first passage time is a standard result [8], while the expression for its variance is new.

Theorem 1. *Let Ω be a bounded domain with smooth boundary $\partial\Omega$ and let Γ be a closed subset of $\partial\Omega$. For each $x \in \Omega$, let τ_x be the first time of a particle hitting Γ, assuming that the particle starts from x, is subject to the Brownian motion in Ω, and reflects from $\partial\Omega$. Then, the mean first passage time, $T(x) := \mathbb{E}[\tau_x]$, and its variance, $v(x) := \mathbb{E}[(\tau_x - T(x))^2]$, are solutions of the following boundary value problems:*

$$-\Delta T = 2 \quad \text{in } \Omega, \qquad T = 0 \quad \text{on } \Gamma, \qquad \partial_n T = 0 \quad \text{on } \partial\Omega \setminus \Gamma; \tag{4}$$

$$-\Delta v = 2|\nabla T|^2 \quad \text{in } \Omega, \qquad v = 0 \quad \text{on } \Gamma, \qquad \partial_n v = 0 \quad \text{on } \partial\Omega \setminus \Gamma. \tag{5}$$

Here $\partial_n := n \cdot \nabla$ is the derivative in the direction n, the exterior normal to $\partial\Omega$.

Moreover, the average of the variance can be calculated from the formula

$$\bar{v} := \frac{1}{|\Omega|}\int_\Omega v(x)\mathrm{d}x = \frac{1}{|\Omega|}\int_\Omega T^2(x)\mathrm{d}x =: \overline{T^2}. \tag{6}$$

The main contribution of this paper is the following closed formula for the mean first passage time in a special case that has attracted much attention and has been the subject of many theoretical investigations in the past; see [1,2,5,9] and the references therein.

Theorem 2. (A Closed Formula) *In two dimensions, with points identified by complex numbers, let*

$$\Omega := \{r\mathrm{e}^{\mathbf{i}\theta} \mid 0 \leqq r < 1, -\varepsilon \leqq \theta \leqq 2\pi - \varepsilon\}, \qquad \Gamma := \{\mathrm{e}^{\mathbf{i}\theta} \mid |\theta| \leqq \varepsilon\}. \tag{7}$$

Then the mean first passage time $T(z)$, for $z \in \bar{\Omega}$, is given by

$$T(z) = \frac{1-|z|^2}{2} + 2\log\left|\frac{1 - z + \sqrt{(1 - z\mathrm{e}^{-\mathbf{i}\varepsilon})(1 - z\mathrm{e}^{\mathbf{i}\varepsilon})}}{2\sin\frac{\varepsilon}{2}}\right|. \tag{8}$$

For the rest of this paper, we will assume Ω and Γ are as in (7). This exact formula allows us to improve the result of Theorem 5.1 in [1] by the following.

Theorem 3. *The mean first passage time T has the following properties:*

$$T(0) = \frac{1}{2} - 2\log\left(\sin\frac{\varepsilon}{2}\right), \qquad \bar{T} := \frac{1}{|\Omega|}\int_\Omega T(x)\mathrm{d}x = T(0) - \frac{1}{4},$$

$$T(\mathrm{e}^{\mathbf{i}\theta}) = 2\,\mathrm{arccosh}\frac{\max\{\sin\frac{\varepsilon}{2}, |\sin\frac{\theta}{2}|\}}{\sin\frac{\varepsilon}{2}} \quad \forall \theta \in \mathbb{R}.$$

In addition, setting $\hat{\varepsilon} = 2\sin\frac{\varepsilon}{2} = |e^{\mathbf{i}\varepsilon} - 1|$, *we have, when* $0 < \hat{\varepsilon} \leqq |1-z|$ *and* $z \in \bar{\Omega}$,

$$T(z) = \frac{1-|z|^2}{2} + 2\log\frac{2|1-z|}{\hat{\varepsilon}} + \Re\left[\frac{z\hat{\varepsilon}^2}{2(1-z)^2}\right] + \frac{O(1)z^2\hat{\varepsilon}^4}{|1-z|^4},$$

where $\Re$ *stands for the real part and* $O(1)$ *is a particular function satisfying* $|O(1)| < 0.887$.

Finally we consider the location of a particle when it exits.

Theorem 4. *The probability density of the location of a particle at time of its exit is given by*

$$\bar{j}(e^{\mathbf{i}\theta}) := -\frac{1}{2\pi}\frac{\partial}{\partial r}T(e^{\mathbf{i}\theta}) = \begin{cases} 0 & \text{if } \varepsilon < \theta < 2\pi - \varepsilon, \\ \dfrac{1}{2\pi}\dfrac{\cos\frac{\theta}{2}}{\sqrt{\sin^2\frac{\varepsilon}{2} - \sin^2\frac{\theta}{2}}} & \text{if } |\theta| < \varepsilon. \end{cases}$$

That is, for any (*Borel set*) $\gamma \subset \partial\Omega$, *the probability that a particle, starting either at the origin or uniformly distributed in* Ω, *making Brownian motion in* Ω, *reflecting when it hits* $\partial\Omega \setminus \Gamma$, *and escaping once it hits* Γ, *so it ends up escaping from* γ *is*

$$P(\gamma) = \int_\gamma \bar{j}(y)\mathrm{d}S_y,$$

where $\mathrm{d}S_y$ *is the surface element of* $\partial\Omega$ *at* $y \in \partial\Omega$.

These Theorems will be proven in the next section.

3. Proof of the Main Results

Proof of Theorem 1. For convenience, we call a particle dead as soon as it hits Γ; otherwise survived. For $x \in \Omega$, we denote by $\rho(x,\cdot,t)$ the survival probability density at time t of the particle starting from x; that is, $\rho(x,y,t)\mathrm{d}y$ is the probability that a particle starting from x lands in the region $y + dy$ at time t before it hits Γ. Then, by the Kolmogrov equation,

$$\begin{cases} \rho_t = \frac{1}{2}\Delta\rho & \text{in } \Omega \times (0,\infty), \\ \rho = 0 & \text{on } \Gamma \times (0,\infty), \\ \partial_n\rho = 0 & \text{on } (\partial\Omega \setminus \Gamma) \times (0,\infty), \\ \rho(x,\cdot,0) = \delta(x-\cdot) & \text{on } \Omega \times \{0\} \end{cases}, \tag{9}$$

where $\delta(x-\cdot)$ is the Dirac mass concentrated at x. If we denote by λ the principal eigenvalue of the operator $-\frac{1}{2}\Delta$ subject to the mixed Neumann (zero on $\partial\Omega \setminus \Gamma$)-Dirichlet (zero on Γ) boundary condition, then

$$0 \leqq \rho(x,y,t) \leqq C e^{-\lambda t} \quad \forall\, y \in \bar{\Omega},\ t \geqq 1,\ x \in \Omega,$$

where C is some positive constant. Since λ is positive, we see that ρ decays exponentially fast in time.

Next we introduce the function

$$G(x, y) := \frac{1}{2}\int_0^\infty \rho(x, y, t)\mathrm{d}t \quad \forall x \in \Omega, y \in \bar{\Omega}.$$

Then it is easy to see that $G(x, \cdot) = 0$ on Γ and $\partial_n G(x, \cdot) = 0$ on $\partial\Omega \setminus \Gamma$. In addition,

$$-\Delta G(x, \cdot) = -\frac{1}{2}\int_0^\infty \Delta\rho(x, \cdot, t)\mathrm{d}t = -\int_0^\infty \rho_t(x, \cdot, t)\mathrm{d}t = \rho(x, \cdot, 0) = \delta(x - \cdot).$$

Thus, G is indeed the Green's function of the Laplace operator Δ associated with the Neumann–Dirichlet boundary condition; that is, for every $x \in \Omega$, $G(x, \cdot)$ is the solution of

$$-\Delta G(x, \cdot) = \delta(x - \cdot) \text{ in } \Omega, \quad G(x, \cdot) = 0 \text{ on } \Gamma, \quad \partial_n G(x, \cdot) = 0 \text{ on } \partial\Omega \setminus \Gamma.$$

Note that the probability that a particle starting from x survives at time t is

$$p(x, t) := \int_\Omega \rho(x, y, t)\mathrm{d}y.$$

Consequently, the probability that a particle dies in the time interval $[t, t + \mathrm{d}t)$ is $p(x, t) - p(x, t + \mathrm{d}t)$. Hence, the expected lifetime (mean first passage time) is given by

$$\begin{aligned} T(x) := \mathbb{E}[\tau_x] &= \int_0^\infty t\Big\{p(x, t) - p(x, t + \mathrm{d}t)\Big\} = -\int_0^\infty t p_t(x, t)\,\mathrm{d}t \\ &= \int_0^\infty p(x, t)\mathrm{d}t = \int_0^\infty \int_\Omega \rho(x, y, t)\mathrm{d}y\mathrm{d}t = \int_\Omega 2\,G(x, y)\mathrm{d}y, \end{aligned}$$

where we have used integration by parts in the third equation. Since G is the Green's function, T is therefore the solution of the mixed Neumann–Dirichlet boundary value problem (4). □

In Monte–Carlo simulations, confidence intervals are estimated in terms of the standard deviation, $\sigma(x)$, of the exit time τ_x, defined by

$$\sigma(x) = \sqrt{v(x)}, \quad v(x) = \mathbb{E}[(\tau_x - T(x))^2] = \mathbb{E}[\tau_x^2] - T(x)^2.$$

To calculate v, we introduce

$$\rho_1(x, y, t) = \int_t^\infty \rho(x, y, s)\mathrm{d}s.$$

Then, for fixed $x \in \Omega$ and $t \geqq 0$, $\rho_1(x, \cdot, t)$ satisfies

$$\rho_1(x, \cdot, t) = 0 \text{ on } \Gamma, \quad \partial_n \rho_1(x, \cdot, t) = 0 \text{ on } \Omega \setminus \Gamma, \quad \rho_1(x, \cdot, 0) = 2G(x, \cdot) \text{ on } \Omega.$$

Also,

$$\frac{1}{2}\Delta\rho_1(x,\cdot,t) = \int_t^\infty \frac{1}{2}\Delta\rho(x,\cdot,s)\mathrm{d}s = \int_t^\infty \rho_s(x,\cdot,s)\,\mathrm{d}s = -\rho(x,\cdot,t)$$
$$= \rho_{1t}(x,\cdot,t) \text{ in } \Omega.$$

Thus,

$$\begin{aligned}
\mathbb{E}[\tau_x^2] &= \int_0^\infty t^2\Big\{p(x,t) - p(x,t+\mathrm{d}t)\Big\} = -\int_0^\infty t^2 p_t(x,t)\mathrm{d}t = \int_0^\infty 2tp(x,t)\mathrm{d}t \\
&= \int_0^\infty 2t\int_\Omega \rho(x,y,t)\mathrm{d}y\mathrm{d}t = -2\int_\Omega\int_0^\infty t\rho_{1t}(x,y,t)\mathrm{d}t\mathrm{d}y \\
&= 2\int_\Omega\int_0^\infty \rho_1(x,y,t)\mathrm{d}t\mathrm{d}y = -\int_0^\infty\int_\Omega \rho_1(x,y,t)\Delta T(y)\mathrm{d}y\mathrm{d}t \\
&= -\int_0^\infty\int_\Omega T(y)\Delta_y\rho_1(x,y,t)\mathrm{d}y\mathrm{d}t = -2\int_\Omega\int_0^\infty T(y)\rho_{1t}(x,y,t)\mathrm{d}t\mathrm{d}y \\
&= 2\int_\Omega T(y)\rho_1(x,y,0)\mathrm{d}y = \int_\Omega 4T(y)G(x,y)\mathrm{d}y.
\end{aligned}$$

This means that $M(x) := \mathbb{E}[\tau_x^2]$ satisfies

$$-\Delta M = 4T \text{ in } \Omega, \qquad M = 0 \text{ on } \Gamma, \qquad \partial_n M = 0 \text{ on } \partial\Omega\setminus\Gamma.$$

Consequently, $v = M - T^2$ is the solution of (5).

Finally, we prove (6) as follows:

$$\begin{aligned}
\bar{v} &:= \frac{1}{|\Omega|}\int_\Omega v(x)\mathrm{d}x = -\frac{1}{2|\Omega|}\int_\Omega v(x)\Delta T(x)\mathrm{d}x = -\frac{1}{2|\Omega|}\int_\Omega T(x)\Delta v(x)\mathrm{d}x \\
&= \frac{1}{|\Omega|}\int_\Omega T(x)|\nabla T(x)|^2\mathrm{d}x = \frac{1}{2|\Omega|}\int_\Omega \nabla T^2(x)\cdot\nabla T(x)\mathrm{d}x \\
&= -\frac{1}{2|\Omega|}\int_\Omega T^2(x)\Delta T(x)\mathrm{d}x = \frac{1}{|\Omega|}\int_\Omega T^2(x)\mathrm{d}s.
\end{aligned}$$

This completes the proof of Theorem 1. □

Remark 3.1. The transition probability density from $W_t = x$ to $W_{t+\Delta t} = y$ for the diffusion process of Brownian motion confined in Ω with reflection boundary $\Omega\setminus\Gamma$ and absorption boundary Γ is $\rho(x,y,\Delta t)$, where ρ is the solution of (9). Thus, the exact discretization of the diffusion process is

$$W_{t+\Delta t} = W_t + \xi_k(W_t) \qquad \forall t \in \mathbf{T} := \cup_{k=0}^\infty\{k\Delta t\},$$

where $\{\xi_k\}_{k=0}^\infty$ are independent random variables and $\xi_k(x)$ has probability density $\rho(x,\cdot,\Delta t)$. Our Monte–Carlo process defined in (1) with $\eta_t \sim N(\mathbf{0},\mathbf{I})$ is just a convenient approximation for $t\in[0,\tau]\cap\mathbf{T}$.

Proof of Theorem 2. We need only show that T given in (8) satisfies (4). For this, we use $\Re(z)$ and $\Im(z)$ to denote the real and imaginary parts of a complex number z. Notice that in default, for $z \in \Omega$ we have

$$\Re\Big(1-z+\sqrt{(1-z\mathrm{e}^{-\mathbf{i}\varepsilon})(1-z\mathrm{e}^{\mathbf{i}\varepsilon})}\Big) = \Re(1-z) + \Re\sqrt{(1-z\mathrm{e}^{-\mathbf{i}\varepsilon})(1-z\mathrm{e}^{\mathbf{i}\varepsilon})} > 0.$$

Hence, taking a real value at $z = 0$, the function

$$f(z) := 2\log\frac{1-z+\sqrt{(1-z\mathrm{e}^{-\mathbf{i}\varepsilon})(1-z\mathrm{e}^{\mathbf{i}\varepsilon})}}{2\sin\frac{\varepsilon}{2}}$$

is analytic in $\bar{\Omega}\setminus\{\mathrm{e}^{\mathbf{i}\varepsilon}, \mathrm{e}^{-\mathbf{i}\varepsilon}\}$ and continuous on $\bar{\Omega}$. Consequently, its real part, $\Re(f)$, is harmonic in Ω. Hence,

$$\Delta T(z) = \Delta\frac{1-|z|^2}{2} + \Delta\Re(f(z)) = \Delta\frac{1-|z|^2}{2} = -2 \quad \forall z \in \Omega.$$

Next, for $z \in \Gamma$, we can write $z = \mathrm{e}^{\mathbf{i}\theta}$ with $|\theta| \leqq \varepsilon$. Then

$$\begin{aligned} f(\mathrm{e}^{\mathbf{i}\theta}) &:= \lim_{r\nearrow 1} 2\log\frac{1-r\mathrm{e}^{\mathbf{i}\theta}+\sqrt{(1-r\mathrm{e}^{\mathbf{i}[\theta-\varepsilon]})(1-r\mathrm{e}^{\mathbf{i}[\theta+\varepsilon]})}}{2\sin\frac{\varepsilon}{2}} \\ &= 2\log\Big[\mathrm{e}^{\mathbf{i}\theta/2}\frac{\sqrt{\sin^2\frac{\varepsilon}{2}-\sin^2\frac{\theta}{2}}-\mathbf{i}\sin\frac{\theta}{2}}{\sin\frac{\varepsilon}{2}}\Big] = \mathbf{i}\Big(\theta - 2\arcsin\frac{\sin\frac{\theta}{2}}{\sin\frac{\varepsilon}{2}}\Big) \\ &\quad \forall\theta \in [-\varepsilon, \varepsilon]. \end{aligned}$$

Thus, $\Re(f(z)) = 0$ when $z \in \Gamma$. Consequently, $T(z) = 0$ on Γ.

Similarly, for $z \in \partial\Omega\setminus\Gamma$, we write $z = \mathrm{e}^{\mathbf{i}\theta}$ with $\theta \in (\varepsilon, 2\pi-\varepsilon)$ to obtain

$$\begin{aligned} \lim_{r\nearrow 1}\arg\sqrt{(1-r\mathrm{e}^{\mathbf{i}[\theta-\varepsilon]}))(1-r\mathrm{e}^{\mathbf{i}[\theta+\varepsilon]})} &= \frac{1}{2}\Big(-\frac{\pi}{2}+\frac{\theta-\varepsilon}{2}\Big) - \frac{1}{2}\Big(\frac{\pi}{2}-\frac{\varepsilon+\theta}{2}\Big) \\ &= \frac{\theta-\pi}{2}. \end{aligned}$$

Hence,

$$\begin{aligned} f(\mathrm{e}^{\mathbf{i}\theta}) := \lim_{r\nearrow 1} f(r\mathrm{e}^{\mathbf{i}\theta}) &= 2\log\Big[\mathrm{e}^{\mathbf{i}(\theta-\pi)/2}\frac{\sin\frac{\theta}{2}+\sqrt{\sin^2\frac{\theta}{2}-\sin^2\frac{\varepsilon}{2}}}{\sin\frac{\varepsilon}{2}}\Big] \\ &= (\theta-\pi)\mathbf{i} + 2\,\mathrm{arccosh}\frac{\sin\frac{\theta}{2}}{\sin\frac{\varepsilon}{2}} \quad \forall\theta \in [\varepsilon, 2\pi-\varepsilon]. \end{aligned}$$

Here $\mathrm{arccosh} : [1,\infty) \to [0,\infty)$ is defined by $\mathrm{arccosh}\, z := \log[z+\sqrt{z^2-1}]$ for $z \geqq 1$. It then follows from the Cauchy Riemann equations, which in the polar coordinates, (r, θ), have the form

$$\frac{\partial}{\partial r}\Re(f(\mathrm{e}^{\mathbf{i}\theta})) = \frac{\partial}{\partial\theta}\Im(f(\mathrm{e}^{\mathbf{i}\theta})) = 1 \quad \forall\theta \in (\varepsilon, 2\pi-\varepsilon). \tag{10}$$

Hence, for $z \in \partial\Omega \setminus \Gamma$,

$$\partial_n T(z) = \frac{\partial}{\partial r}\frac{1-|z|^2}{2} + \frac{\partial}{\partial r}\Re(f(z)) = 0.$$

Therefore, by the uniqueness of the solution of problem (4), T is given by the formula (8). This completes the proof of Theorem 2. □

Proof of Theorem 3. The formula $T(0)$ and $T(e^{\mathbf{i}\theta})$ follows directly from (8) and the calculation of $f(e^{\mathbf{i}\theta})$ in the proof of Theorem 2. Also, by the Mean Value Theorem for harmonic functions,

$$\bar{T} = \frac{1}{|\Omega|}\int_\Omega \frac{(1-|x|^2)}{2}\mathrm{d}x + \Re f(0) = \frac{1}{4} + 2\log\frac{1}{\sin\frac{\varepsilon}{2}} = T(0) - \frac{1}{4}.$$

For the asymptotic (indeed, Taylor) expansion, we can write T in (8) as

$$\begin{aligned} T(z) &= \frac{1-|z|^2}{2} + 2\log\frac{|1-z|}{\sin\frac{\varepsilon}{2}} + 2\Re\log\frac{1+\sqrt{1+b^2}}{2}, \\ b &:= \frac{2\sqrt{z}\sin\frac{\varepsilon}{2}}{1-z} = \frac{\sqrt{z}\hat{\varepsilon}}{1-z}. \end{aligned}$$

When $0 < \hat{\varepsilon} \leqq |1-z|$ and $z \in \bar{\Omega}$, we have $|b| < 1$. Applying the maximum principle for the analytic function $\zeta^{-2}\{\log\frac{1+\sqrt{1+\zeta}}{2} - \frac{\zeta}{4}\}$ on the unit disc we find that

$$\left|\log\frac{1+\sqrt{1+\zeta}}{2} - \frac{\zeta}{4}\right| \leqq \left(\ln 2 - \frac{1}{4}\right)|\zeta|^2 \leqq 0.4432|\zeta|^2 \quad \forall\, |\zeta| \leqq 1.$$

The stated expansion for T thus follows. □

Remark 3.2. (1) It is clear from (8) that the function T is smooth (C^∞) in $\bar{\Omega} \setminus \{e^{\mathbf{i}\theta}, e^{-\mathbf{i}\theta}\}$ and Hölder continuous with exponent $\frac{1}{2}$ on $\bar{\Omega}$.

(2) The constant $\bar{T}$ is the average of the mean exit time. It was derived in [4,9] in the case of one absorbing window, and in [5] for the case of a cluster of small absorbing windows that

$$\bar{T} = 2\log\frac{2}{\varepsilon} + O(1).$$

In [1, Theorem 5.1], it was rigorously shown that

$$\bar{T} = \frac{1}{4} - 2\log\left(\sin\frac{\varepsilon}{2}\right) + O(1)\varepsilon.$$

Clearly, our formula shows that the above $O(1)$ term is, indeed, exactly zero.

Proof of Theorem 4. The flux $\bar{j}$ is calculated by using

$$\frac{\partial}{\partial r}T(e^{\mathbf{i}\theta}) = -1 + \frac{\partial}{\partial\theta}\Im(f(e^{\mathbf{i}\theta}))$$

and the expression of $f(e^{\mathbf{i}\theta})$.

Note that for $x \in \Omega$, the quantity $-\frac{1}{2}n(y)\cdot\nabla_y\rho(x, y, t)\mathrm{d}S_y\mathrm{d}t$ is the probability that a particle starting from x ends up escaping from $\mathrm{d}S_y$ in time interval $[t, t+\mathrm{d}t)$. Hence, the probability that a particle starting from x ends up escaping from $\mathrm{d}S_y$ is $j(x, y)\mathrm{d}S_y$, where

$$j(x, y) = -\frac{1}{2}\int_0^\infty n(y)\cdot\nabla_y\rho(x, y, t)\mathrm{d}t = -n(y)\cdot\nabla_y G(x, y).$$

(1) First we consider the case in which the particle is initially at $x = 0$. Then direct computation shows that

$$G(0, z) = -\frac{1}{2\pi}\log|z| + \frac{|z|^2 - 1}{4\pi} + \frac{T(z)}{2\pi}.$$

Consequently,

$$j(0, e^{\mathbf{i}\theta}) = -\frac{\partial}{\partial r}G(0, re^{\mathbf{i}\theta})|_{r=1} = -\frac{1}{2\pi}\frac{\partial}{\partial r}T(e^{\mathbf{i}\theta}) = \bar{j}(e^{\mathbf{i}\theta}).$$

Thus, $\bar{j}$ *is the escaping probability density of particles starting from the origin.*

(2) Next assume that the initial position of a particle is uniformly distributed in Ω. Then the probability that the particle exits from $\mathrm{d}S_y$ is

$$\begin{aligned}\frac{1}{|\Omega|}\int_\Omega\Big(j(x, y)\mathrm{d}S_y\Big)\,\mathrm{d}x &= -\frac{\mathrm{d}S_y}{|\Omega|}\int_\Omega\Big(n(y)\cdot\nabla_y G(x, y)\Big)\mathrm{d}x\\ &= -\frac{\mathrm{d}S_y}{|\Omega|}n(y)\cdot\nabla_y\int_\Omega G(y, x)\mathrm{d}x\\ &= -\frac{\mathrm{d}S_y}{2|\Omega|}n(y)\cdot\nabla_y T(y)\\ &= \bar{j}(y)\mathrm{d}S_y \qquad \forall\, y \in \partial\Omega.\end{aligned}$$

Thus, $\bar{j}$ *is also the escaping probability density of particles initially uniformly distributed in* Ω. This completes the proof. □

4. Monte–Carlo Simulations

The Discretization We simulate the confined Brownian motion by n sample paths, $P_1, \ldots, P_n$. The sample path P_i is described by $\{X_i^{k\Delta t}\}_{k=0}^\infty$ where $X_i^{k\Delta t}$ represents the position of the particle at time $t = k\Delta t$. Here $\{X_i^{k\Delta t}\}$ are random variables sequentially defined by

$$X_i^0 = \eta_{i0}, \quad Y_i^k := X_i^{(k-1)\Delta t} + \eta_{ik}\sqrt{\Delta t}, \quad X_i^{k\Delta t} = \frac{Y_i^k}{\max\{1, |Y_i^k|^2\}},$$
$$i = 1, \ldots, n,\ k = 1, 2, \ldots,$$

where $\{\eta_{10}, \ldots, \eta_{n0}\}$ are the starting positions related to the initial distribution of the particle, and $\{\eta_{ik} | i = 1, \ldots, n,\ k = 1, 2, \ldots\}$ are independent and identically distributed random variables with mean vector $(0, 0)$ and covariance matrix equal to identity. Note that Y_i^k is the position at time $k\Delta t$ of the discretized Brownian particle if it were not bouncing from $\partial\Omega$. In our computations, we represent bouncing from the boundary $\partial\Omega$ by the Kelvin transformation $z \longrightarrow z/|z|^2$ for $|z| > 1$. Other reflection principles can also be used; for example, one can return the particle to the position it occupied before it took the final step causing reflection, or one can reflect the particle geometrically from the boundary without significant change in the results, provided the step size is small. If we are simulating particles starting from a fixed point $z \in \Omega$, we simply take $\eta_{i0} = z$ for $i = 1, \ldots n$. In the computations below we take all particles starting from the center, $z = 0$. For exit times from random points, one can generate random starting points from common random numbers (CRNs).

As long as $\{\eta_{ik}\}$ are independent and identically distributed random variables with mean vector $(0, 0)$, covariance matrix $\mathbf{I}$ and finite fourth order momentum, the limit, as $\Delta t \searrow 0$, of the piecewise linear curve connected by points $\{(k\Delta t, X_i^{k\Delta t})\}_{k=0}^{\infty}$ is a Brownian motion path. There are two standard choices of the independent and identically distributed random variables $\{\eta_{ik}\}$:

(i) $\{\eta_{ik} \mid i = 1, \ldots, n,\ k = 1, 2, \ldots\}$ are independent and identically distributed random variables with a $\frac{1}{4}$ probability of moving either southeast, southwest, northeast, or northwest, with distance $\sqrt{2}$.
(ii) $\{\eta_{ik} \mid i = 1, \ldots, n,\ k = 1, 2, \ldots\}$ are independent and identically distributed random variables with $N((0, 0), \mathbf{I})$ Gaussian distribution. This is the method we use. It has the advantage that we can run statistics for any $\Delta t > 0$.

Numerically, it may be preferable to use $\Delta x := \sqrt{\Delta t}$ as a parameter to address the accuracy of the approximation of the Brownian motion by discretization.

The First Hitting Time For the ith particle path, $\{X_i^{k\Delta t}\}_{k=0}^{\infty}$, its time of first hitting Γ is defined as

$$T_i := k_i \Delta t, \qquad k_i := \min\{k \in \mathbb{N} \mid \arg(X_i^{k\Delta t}) \in [-\varepsilon, \varepsilon], |Y_i^k| \geqq 1\}.$$

We terminate the simulation for the ith particle when we reach the time T_i. Figure 1 shows four histograms of the first exit times $\{T_i\}_{i=1}^n$, in Monte–Carlo simulations with $n = 400{,}000$, $\Delta x = \pi/256$, and gate size $\varepsilon = \pi, \pi/2, \pi/8$, and $\pi/128$, respectively.

The Randomness Error In a given Monte–Carlo simulation, $\{\eta_{ik}\}$ are generated from CRNs according the needed distribution. The sample mean and sample standard deviation are calculated by

$$\hat{T} = \frac{1}{n}\sum_{i=1}^{n} T_i, \qquad \hat{\sigma} = \left\{\frac{1}{n-1}\sum_{i=1}^{n}(T_i - \hat{T})^2\right\}^{1/2}.$$

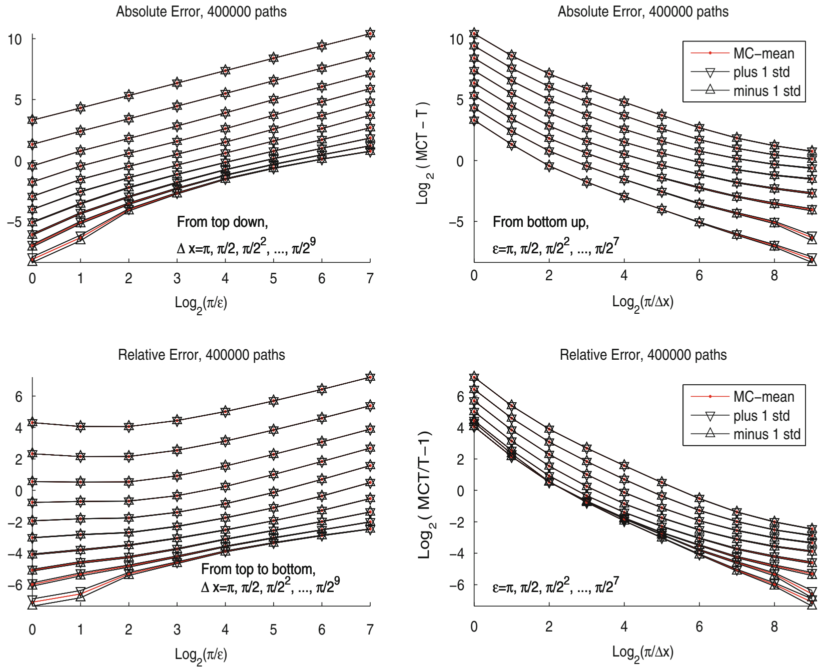

Fig. 2. Absolute error and relative error in the $\log_2$ scale, with respect to ε and Δx. Here $\mathrm{MCT} = \hat{T}$ represents the mean escape time from Monte–Carlo simulation. The *triangular marks* are those for $\mathrm{MCT} = \hat{T} + \hat{\sigma}/\sqrt{n}$ and $\mathrm{MCT} = \hat{T} - \hat{\sigma}/\sqrt{n}$ respectively. When $\Delta x/\varepsilon \leqq 2^{-9}$, statistical errors (from $n = 400{,}000$ sample paths) begin to mess up the plot

Denote by $T_{\Delta t} = \lim_{n\to\infty} \hat{T}$. Then by the Central Limit Theorem, for $n \geqq 10$, we can present our conclusion from a Monte–Carlo simulation as $\hat{T} \approx T_{\Delta t} + N(0, \hat{\sigma}^2/n)$, or simply

$$T_{\Delta t} = \hat{T} \pm \frac{\hat{\sigma}}{\sqrt{n}} \quad \text{with 65\% confidence,} \qquad T_{\Delta t} = \hat{T} \pm \frac{3\hat{\sigma}}{\sqrt{n}} \quad \text{with 99\% confidence.}$$

In our simulations, we take $n = 400{,}000$ particles, so the Central Limit Theorem can be reasonably applied (recalling from the proof of Theorem 1 that the probability distribution density of τ_x has an exponential tail). Our simulation (starting from $(0, 0)$) shows that $\hat{\sigma}$ is proportional to $\hat{T}$ with proportional constant almost equal to 1 (Fig. 1).

Discretization Error Using the approximation $T_{\Delta t} \approx \hat{T} \pm \hat{\sigma}/\sqrt{n}$, we display the absolute error $T_{\Delta t} - T$ (> 0) and relative error $T_{\Delta t}/T - 1$ in Figs. 2 and 3. From the Figures, one sees that $\log_2(T_{\Delta t} - T)$ is almost linear in $\log_2 \varepsilon$ and in $\log_2 \Delta x$. This suggests that

$$T_{\Delta t} - T \approx \frac{2\Delta x}{\varepsilon}, \qquad \frac{T_{\Delta t}}{T} - 1 \approx \frac{4\Delta x}{\varepsilon(1 + 4|\ln \sin \frac{\varepsilon}{2}|)}.$$

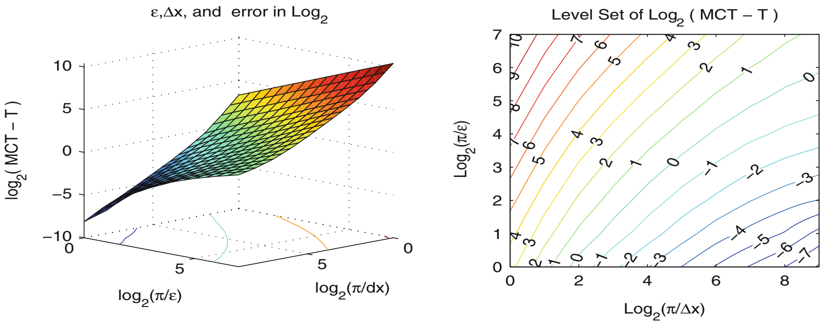

Fig. 3. Variation of error with respect to ε and Δx. In the region $\varepsilon > \Delta x$, each level set can be regarded as a line of slop 1, so that $\log_2(T_{\Delta t} - T) \approx 1 + \log_2(\pi/\varepsilon) - \log_2(\pi/\Delta x)$, rendering $T_{\Delta t} - T \approx 2\Delta x/\varepsilon = 2\sqrt{\Delta t}/\varepsilon = 4\sqrt{\Delta t}/|\Gamma|$

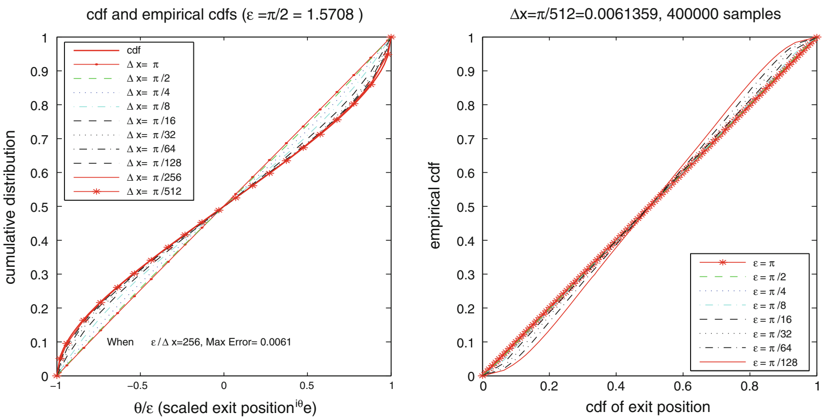

Fig. 4. *Left* cdf(θ) and ecdf(θ) against θ/ε, for fixed ε and various Δx. *Right* Parametric curves $\{(\mathrm{cdf}(\theta), \mathrm{ecdf}(\theta)) \mid \theta \in [-\varepsilon, \varepsilon]\}$ for fixed Δx and various ε. When $\Delta x \leqq \varepsilon/64$, the cdf and ecdf are almost indistinguishable

Distribution of Exits Using the positions of the sample exits $\{X_i^{T_i}\}_{i=1}^n \subset \Gamma$, we can find the sample distribution of the exits along the gate and compare it with the theoretical density $\bar{j}(y)$, $y \in \Gamma$ from Theorem 4. For fixed ε, we compare the empirical cumulative distribution function

$$\mathrm{ecdf}(\theta) := \frac{1}{n} \sum_{\arg(X_i^{T_i}) \in [-\varepsilon, \theta]} 1 \quad ,$$

for various different Δx, with the true

$$\mathrm{cdf}(\theta) = \mathbb{P}\Big(\arg(W_\tau) \in (-\varepsilon, \theta)\Big) = \int_{-\varepsilon}^{\theta} \bar{j}(s)\mathrm{d}s = \frac{1}{2} + \frac{1}{\pi} \arcsin \frac{\sin\frac{\theta}{2}}{\sin\frac{\varepsilon}{2}}$$
$$\forall \theta \in [-\varepsilon, \varepsilon],$$

where τ is the first hitting time of the confined Brownian motion $\{W_t\}$, which starts from the origin and bounces from the unit circle. For fixed Δx and various ε (noting that cdf depends on ε), we consider the uniformly distributed random variable $\mathrm{cdf}(\arg(W_\tau))$. This is equivalent to plotting cdf–ecdf graphs. The results are shown in Fig. 4.

Acknowledgments. C.C. thanks the Brackenridge Fellowship of the University of Pittsburgh for its support. The support for X.C. through NSF grant #10008905 is gratefully acknowledged.

References

1. Chen, X., Friedman, A.: *Asymptotic Analysis for the Narrow Escape Problem*, Preprint.
2. Cheviakov, A.F., Ward, M.J., Straube, R.: An asymptotic analysis of the mean first passage time for narrow escape problems. Part II: the sphere. *SIAM Multiscale Model. Simul.* (to appear)
3. Grigoriev, I.V., Makhnovskii, Y.A., Berezhkovskii, A.M., Zitserman, V.Y.: Kinetics of escape through a small hole. *J. Chem. Phys.* **116**, 9574–9577 (2002)
4. Holcman, D., Schuss, Z.: Escape through a small opening: receptor trafficking in a synaptic membrane. *J. Stat. Phys.* **117**, 975–1014 (2004)
5. Holcman, D., Schuss, Z.: Diffusion escape through a cluster of small absorbing windows. *J. Phys. A: Math. Theory* **41**, 155001 (2008)
6. Pillay, S., Ward, M.J., Peirce, A., Kolokolnikov, T.: An asymptotic analysis of the mean first passage time for narrow escape problems. Part I: two dimensional domains. *SIAM Multiscale Model. Simul.* (to appear)
7. Redner, S.: *A Guide to First Passage Time Processes*. Cambridge University Press, 2001
8. Schuss, Z.: *Theory and Applications of Stochastic Differential Equations: An Analytical Approach*. Springer, New York, 2010
9. Singer, A., Schuss, Z., Holcman, D.: Narrow escape. Part II: the circular disk. *J. Stat. Phys.* **122**, 465–489 (2006)
10. Zwanzig, Z.: A rate process with an entropy barrier. *J. Chem. Phys.* **94**, 6147–6152 (1991)

Department of Mathematics,
University of Pittsburgh,
Pittsburgh, PA
15260, USA.
e-mail: xinfu@pitt.edu

and

Present Address:
Applied Mathematics,
Brown University,
Box F, 182 George Street,
Providence, RI
02912, USA.
e-mail: carey_caginalp@brown.edu

(*Received September 10, 2010 / Accepted July 25, 2011*)
Published online September 24, 2011 – *© Springer-Verlag* (*2011*)