Enhanced diffusion through surface excursion: A master-equation approach to the narrow-escape-time problem

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We present a master-equation approach to the narrow-escape-time (NET) problem, i.e., the time needed for a particle contained in a confining domain with a single small or narrow opening to exit the domain. In this paper we introduce an alternative type of confining domain (to the usually spherical one) and we consider the diffusion process on a lattice rather than in continuous space. We have obtained analytic results for the basic quantity studied in the NET problem, the mean first-passage time, and we have studied its dependence in terms of the transition (desorption) probability over (from) the surface boundary and the confining domain dimensions. In addition to our analytical approach, we have implemented Monte Carlo simulations, finding excellent agreement between the theoretical results and simulations.

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I. INTRODUCTION

Intermittent processes are widespread in many domains and fields. Generally speaking, these processes involve an agent (particle, searcher, etc.) and two or more phases among which it alternates. The term "phase" must be understood in a broad sense, since, depending on the context, it may involve different ways of propagation, as is the case of an intermittent search where active search phases (e.g., Brownian motion phases) randomly alternate with fast relocation phases (e.g., ballistic motion phases) [1], and different interfaces, as may be the situation of a reactant that freely diffuses in a solvent and intermittently binds to a cylinder [2], etc. We also find this sort of intermittent behavior in the binding of a protein to specific sites on DNA for regulating transcription [3–5]. In interface sciences (see Refs. [6,7] and references therein) the adsorption-desorption dynamics of molecules are of fundamental importance and are crucial to a number of technologies. These include solutions or melts of synthetic macromolecules [8,9], colloidal dispersions [10], and in the manufacture of self-assembled monolayers and multilayers [11,12].

Among these kinds of processes we find the so-called *narrow-escape-time* problem (NET), i.e., the time needed for a particle contained in a confining domain with a single small opening to exit the domain. The NET problem is prominent in cellular biology, since it is related to the random time needed by a particle (released inside the cell) to activate a given mechanism on the cell membrane, for example, the particle may be a protein that looks for a specific site on a DNA string [3–5]. Since the seminal work of Berg and Purcell [13], the research in the area has experienced steady growth over time and has motivated a great deal of work [14–25].

Recently, different approaches were made to the NET problem. For instance, in Ref. [23] a mean-field approximation to calculate the mean reaction (search) time is developed, and in Ref. [24] a backward equation-type formalism is presented. In all cases very interesting results and conclusion are presented.

The aim of this paper is to present a model we believe is both simple enough to be studied analytically, and rich enough to show the impact of geometrical parameters in the system and to show the interplay between surface and boundary paths. In this paper we introduce a rectangular-shaped confining domain (since the importance of two-dimensional regions for the NET problem has been well established [26]), and we consider the diffusion process on a lattice rather than in continuous space.

In order to perform our research we exploit Dyson's [6] theory. We use the concept of *mean first-passage time* (MFPT), and we establish the connection with the *first-passage time* (FPT) corresponding to the problem of a single walker.

The outline of this paper is as follows. In the following section we introduce our model and provide the basic definitions and concepts. We also describe the proposed analytical approach and present the main results. Section III depicts several assorted illustrations for the MFPT to the target site for different configurations of the system through a comparison between our analytical framework and Monte Carlo (MC) simulations. In Sec. IV we discuss our conclusions and perspectives. Finally, in the Appendix we briefly discuss, through MC simulations, a more general confining domain.

II. ANALYTICAL APPROACH

A. The model

Let us start with the problem of a walker making a random walk in a finite rectangular $N \times (M+1)$ lattice (see Fig. 1). The surface is bounded in the y direction, where the walkers can move from $y = 0$ to $y = M$, and periodic boundary conditions are assumed in the x direction so x and $x + N$ denote the same place in space. A perfect trap is located at point (0,0), so a walker reaching that place is caught with probability one. We follow the walker evolution through the system considering the conditional probability $P(n,m,t|n_0,m_0,t=0) \equiv P(n,m,t)$, that is, the probability that an "unrestricted" walker is at (n,m) [where (n,m) are discrete coordinates in the (x,y) space] at time t given that

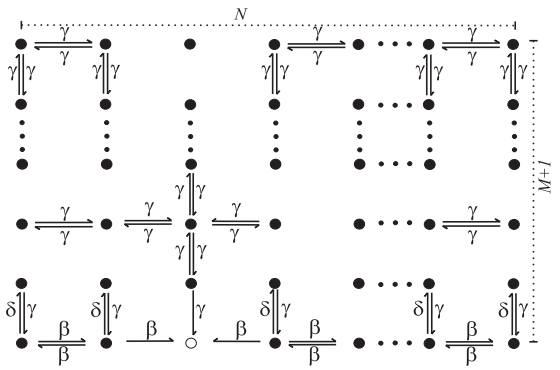

FIG. 1. Schematic transitions of the walker to or from the baseline and to or from a generic surface site. Notice that the trap site (open circle) could be reached both from the surface (with transition rate γ) and from the baseline (with transition rate β).

it was at $(n_0;m_0)$ at $t=0$. By "unrestricted" we identify a situation with no traps or sinks present in the system. $P(n,m,t)$ satisfies the following master equation:

$$\begin{aligned}
\dot{P}(n,0,t) &= \gamma P(n,1,t) - \delta P(n,0,t) \\
&\quad + \beta(P(n+1,0,t) + P(n-1,0,0,t) \\
&\quad - 2P(n,0,t)), \quad m=0, \\
\dot{P}(n,1,t) &= \delta P(n,0,t) - 4\gamma P(n,1,t) \\
&\quad + \gamma(P(n+1,1,t) + P(n-1,1,t) \\
&\quad + P(n,2,t)), \quad m=1, \\
\dot{P}(n,m,t) &= \gamma(P(n-1,m,t) + P(n+1,m,t) \\
&\quad + P(n,m+1,t) + P(n,m-1,t)) \\
&\quad - 4\gamma P(n,m,t), \quad 2 \leqslant m \leqslant M-1, \\
\dot{P}(n,M,t) &= \gamma(P(n-1,M,t) + P(n+1,M,t) \\
&\quad + P(n,M-1,t)) \\
&\quad - 3\gamma P(n,M,t), \quad m=M,
\end{aligned} \tag{1}$$

where γ is the surface transition probability per unit time in the x and y directions, β is the transition probability over the line $m=0$ in the x direction, and δ is the desorption probability per unit time from the boundary line $m=0$.

In what follows, we will denote an integral transform by its argument. Thus, for example, the Laplace transform on t and the (finite) Fourier transform on a coordinate (e.g., x) would read

$$\begin{aligned}
P(k,m,u|n_0,m_0,0) &\equiv \mathcal{F}\{\mathcal{L}[P(k,m,t|n_0,m_0,0)]\} \\
&= \sum_{n=0}^{N-1} e^{ikn} \int_0^\infty e^{-ut} P(n,m,t|n_0,m_0,0)\, dt.
\end{aligned}$$

As we are interested in the MFPT through the trap site, let us define $F(0,0,t|n_0,m_0,0)$ as the first-passage time density (FPTD) through the site (0,0) at time t, given that the walker was at (n_0,m_0) at time $t=0$. The connection between FPTD and the "unrestricted" conditional probability $P(n,m,t|n_0,m_0,t=0)$ is established through the "renewal approach" [27]. This approach in the Laplace domain gives

$$F(0,0,u|n_0,m_0,t=0) = \frac{P(0,0,u|n_0,m_0,t=0)}{P(0,0,u|0,0,t=0)}, \tag{2}$$

which is the known Siegert's formula [28].

Following the guidelines of Ref. [27], we can evaluate the MFPT through the trap site (0,0) as

$$\begin{aligned}
T &= \int_0^\infty t \sum_{n_0,m_0} F(0,0,t|n_0,m_0,0) g(n_0,m_0)\, dt \\
&= -\frac{\partial}{\partial u} \left\{ \sum_{n_0,m_0} F(0,0,u|n_0,m_0,0) g(n_0,m_0) \right\} \Bigg|_{u=0},
\end{aligned} \tag{3}$$

where $g(n,m)$ denotes the probability density of initially finding the walker at a position (n,m).

B. Matrix formalism and analytical results

Let us focus on the probability $P(n,m,t|n_0,m_0,t=0)$, which is the building block for the MFPT. Taking the (finite) Fourier transform with respect to the x variable and the Laplace transform with respect to the time t in Eq. (1), we obtain

$$\begin{aligned}
&m=0, \\
&uP(k,0,u) - P(k,0,t=0) \\
&\quad = \gamma P(k,1,u) - [\delta - A_1(k)] P(k,0,u), \\
&m=1, \\
&uP(k,1,u) - P(k,1,t=0) \\
&\quad = \delta P(k,0,u) + \gamma P(k,2,u) - [2\gamma - A(k)] P(k,1,u), \\
&2 \leqslant m \leqslant M-1, \\
&uP(k,m,u) - P(k,m,t=0) \\
&\quad = A(k) P(k,m,u) + \gamma(P(k,m+1,u) + P(k,m-1,u), \\
&\quad\quad -2P(k,m,u)) \\
&m=M, \\
&uP(k,M,u) - P(k,M,t=0) \\
&\quad = A(k) P(k,M,u) + \gamma P(k,M-1,u) - \gamma P(k,M,u).
\end{aligned} \tag{4}$$

Here we have defined $A_1(k) = 2\beta(\cos k - 1)$, $A(k) = 2\gamma(\cos k - 1)$.

Using the matrix formalism, Eq. (4) can be written as

$$[u\mathbb{I} - \mathbb{H}]\,\mathbb{P} = \mathbb{I}\,, \tag{5}$$

where $\mathbb{I}$ is the identity matrix, $\mathbb{H}$ is an $(M+1)\times(M+1)$ tridiagonal matrix with elements

$$\mathbb{H} = \begin{bmatrix}
C_1 & \gamma & 0 & \dots & \dots & 0 \\
\delta & C & \gamma & 0 & \dots & 0 \\
0 & \gamma & C & \gamma & 0 & \vdots \\
\dots & 0 & \ddots & \ddots & \ddots & \vdots \\
\dots & \dots & \dots & \gamma & C & \gamma \\
0 & \dots & & 0 & \gamma & \gamma + C
\end{bmatrix}, \tag{6}$$

where C and C_1 are defined as $C = -2\gamma + A(k)$, $C_1 = -\delta + A_1(k)$, and $\mathbb{P}$ is an $(M+1)\times(M+1)$ matrix with components

$$[\mathbb{P}(k,u)]_{m,m_0} = P(k,m,u|n_0,m_0,t=0)\,.$$

In order to find the solution to Eq. (5) we decompose the $\mathbb{H}$ matrix in the following way:

$$\mathbb{H} = A(k)\mathbb{I} + \mathbb{H}^0 + \mathbb{H}^1 + \mathbb{H}^2, \tag{7}$$

where

$$\mathbb{H}^0 = \begin{bmatrix} -\gamma & \gamma & 0 & \dots & 0 \\ \gamma & -2\gamma & \gamma & \dots & 0 \\ 0 & \gamma & -2\gamma & \gamma & 0 \\ \dots & \dots & \dots & \dots & \\ \dots & \dots & \gamma & -2\gamma & \gamma \\ \dots & & 0 & \gamma & -\gamma \end{bmatrix} \tag{8}$$

corresponds to the transition matrix for a symmetric random walk to nearest neighbors in a finite lattice ($M+1$ sites) with reflective boundary conditions at the ends. On the other hand,

$$\mathbb{H}^1 = [\gamma - \delta + A_1(k) - A(k)]\delta_{i,0}\delta_{0,j}, \tag{9}$$

$$\mathbb{H}^2 = -(\gamma - \delta)\,\delta_{i,1}\,\delta_{0,j}. \tag{10}$$

A formal solution to Eq. (5) is

$$\mathbb{P} = [u\mathbb{I} - \mathbb{H}]^{-1}. \tag{11}$$

By applying the Dyson procedure [6] a general expression for $[\mathbb{P}(k,u)]_{m,m_0}$ can be found. From this, the probability that a walker is on the surface at site (n,m) at time t given it was at (n_0,m_0) at $t=0$, $P(n,m,t|n_0,m_0,t=0)$ is derived by using the inverse Laplace transform on u and the inverse Fourier transform on k (for the x coordinate) for each matrix element $[\mathbb{P}(k,u)]_{m,m_0}$. Notice that, as we are interested in the calculation of (3), we only need to perform the inverse Fourier transform on $P(0,0,u|n_0,m_0,t=0)$ i.e., we need the elements $\mathcal{F}^{-1}\{[\mathbb{P}(k,u)]_{0,m_0}\}$. In this case it can be shown that

$$[\mathbb{P}(k,u)]_{0,m_0} = \frac{\eta^{m_0} + \eta^{\tilde{M}-m_0}}{\delta(1-\eta)(1-\eta^{\tilde{M}-1}) + [u - A_1(k)](1+\eta^{\tilde{M}})}, \tag{12}$$

where $\eta = 1 + (\tilde{u} - \sqrt{\tilde{u}^2 + 4\gamma\tilde{u}})/2\gamma$, $\tilde{M} = 2M+1$ and $\tilde{u} = u - A(k)$. The inverse Fourier transform on $[\mathbb{P}(k,u)]_{0,m_0}$ is carried out in the following way:

$$P(0,0,u|n_0,m_0,t=0) = \frac{1}{N}\sum_{q=0}^{N-1} e^{i\frac{2\pi n_0 q}{N}} \left[\mathbb{P}\left(\frac{2\pi q}{N},u\right)\right]_{0,m_0}. \tag{13}$$

So far we have obtained the required expression for the calculation of the MFPT through the target site. Let us move on and evaluate the MFPT for a walker with an initial uniform distribution on the baseline ($y=0$), i.e., $g(n,m) = (1-\delta_{n,0})\delta_{m,0}/(N-1)$ [notice that we explicitly exclude the possibility of having a walker at (0,0) at $t=0$]. We obtain

$$T = \frac{N}{N-1}\frac{\delta M + \gamma}{\gamma}\sum_{q=1}^{N-1}\left[\mathbb{P}\left(\frac{2\pi q}{N},u=0\right)\right]_{0,0}. \tag{14}$$

Equation (14) constitutes one of our main results and an interesting physical insight can be extracted from it. First it can be shown that $\eta^M \simeq 0$ [29], considering $N/(N-1) \simeq 1$ and calling $z_q = 1 - \cos\frac{2\pi q}{N}$, Eq. (14) can be expressed as

$$T \simeq \frac{\delta M + \gamma}{\gamma}\sum_{q=1}^{N-1}\frac{1}{(2\beta-\delta)z_q + \delta\sqrt{z_q^2 + 2z_q}}. \tag{15}$$

Now consider the regimes (i) $\delta \ll 2\beta$ (particularly $\delta \ll \gamma$), (ii) $\delta \approx 2\beta$, and (iii) $\delta \gg 2\beta$ (particularly $\delta \gg \gamma$). In (i) the sum on the right-hand side takes the form $\sim\sum z_q^{-1}$. Notice that the main contribution to this sum comes from the $z_q \sim 0$ neighborhood, i.e., from $1-\cos\frac{2\pi q}{N} \simeq \frac{1}{2}(\frac{2\pi q}{N})^2$, so $\sum z_q^{-1} \sim N^2$. Taking into account these considerations, a first-order approximation gives $T \sim a_1\frac{N^2}{2\beta}$, where a_1 is a computable parameter. In (ii) and (iii) a similar argument could be used. The difference is that, in this case, $\sim\sum z_q^{-1/2} \sim N$, then in (ii) $T \sim a_2(\gamma^{-1}MN + (2\beta)^{-1}N)$ and in (iii) $T \sim a_3\gamma^{-1}MN$. As before a_2 and a_3 are computable parameters. In the following scheme we summarize the three regimes:

$$T \sim \begin{cases} (2\beta)^{-1}N^2 & \text{if } \delta \ll 2\beta, \\ \gamma^{-1}MN + (2\beta)^{-1}N & \text{if } \delta \approx 2\beta, \\ \gamma^{-1}MN & \text{if } \delta \gg 2\beta. \end{cases} \tag{16}$$

Equation (16) deserves further discussion. The literature [30,31] shows that in finite systems the MFPT behaves $\sim L^D$, where D is the space dimension and L is a length characteristic of the system. Consider first the regimes (ii) and (iii). In (ii) when $\delta \approx 2\beta$, we have a *mixed* type of transport. Contributions to this regime arise from "surface journeys" ($\sim MN$) and "boundaries pathways" ($\sim N$). In the $\delta \gg 2\beta$ regime, however, any surface pathway is preferred to a boundary path and $T \sim \gamma^{-1}MN$. Regime (i) deserves special attention since in this case $\delta/\gamma \ll 1$ (i.e., once in the baseline the walker has an extremely low desorption probability), and according to the initial distribution (the walker starts it journey on the baseline) one may assume that the MFPT would scale as $\sim N$, however, a $\sim N^2$ scaling is obtained. This behavior arises from the chosen initial distribution; as we discussed earlier, this regime is equivalent to a one-dimensional (1D) motion, so here [31] $T_{n_0} = n_0(N-n_0)/2\beta$, which computes the arrival time to site 0 starting from n_0. Averaging T_{n_0} over starting sites (uniform initial distribution) results in $T = \sum_{n_0} T_{n_0}/(N-1) = \frac{1}{6}\frac{(N^3-N)}{2\beta(N-1)} \sim N^2/2\beta$, which accounts for the observed result.

The transition between regimes can be understood studying the mean return time, a value related to the system size in the y direction and the desorption probability. In particular, for our confining domain we evaluate the mean return time [32] to the baseline (not necessarily to the trap) and get

$$T_{\text{ret}} = \frac{1}{\delta} + \frac{M}{\gamma}. \tag{17}$$

T_{ret} represents the time needed to leave the baseline ($1/\delta$) and return to it (M/γ). If we have N possible destination sites on the baseline, we would expect the mean time to hit a specific site, i.e., the MPFT to that site, behave like $T \sim NT_{\text{ret}} = \delta^{-1}N + \gamma^{-1}MN$. Notice that with this rather informal argument we have reobtained the MFPT in regime (ii) of (16). The role of T_{ret} is highlighted in the following closed expression for Eq. (15) (in the limit $z_q \sim 0$):

$$T \simeq \left[\frac{1}{\delta} + \frac{M}{\gamma}\right]\frac{N}{\pi}\left[\gamma_e + \Psi(N) + \Psi\left(1 + \frac{N\delta}{\pi(2\beta-\delta)}\right) - \Psi\left(N + \frac{N\delta}{\pi(2\beta-\delta)}\right)\right], \tag{18}$$

where $\Psi(z)$ is the digamma function and γ_e is the Euler's constant [33]. The mean return time can be seen in the first

factor on the right-hand side of Eq. (18). Notice the similarity between Eqs. (18) and (6) in Ref. [24].

III. ILLUSTRATIONS

Here we illustrate the general framework introduced in the previous section and compare our theoretical results to independent Monte Carlo simulations. In the next figures, lines indicate analytical calculations and symbols correspond to Monte Carlo (MC) simulations. All times are given in units of the inverse of the surface transition probability $(1/\gamma)$.

In Fig. 2 we present curves corresponding to the MFPT, T, as a function of the desorption rate δ, with $N = 20$, $M = 10$ (inset: $M = 30$), for different values of the transition rate over the baseline β. Notice how β strongly influences the regime $\delta/\gamma \ll 1$. In this case, and taking into account the walker's initial distribution, the transport is performed on the baseline (lower boundary) of the confining domain, so this is an expected behavior. On the other hand, this influence is, as expected, considerably less when $\delta \gg 2\beta$ since in this regime surface excursions are favorable. As can be inferred from the figure, the transition rate β plays an important role as it seems to regulate, for fixed values of N and M, the existence of an optimal value for δ. It is worth remarking that the same β values that contribute to a minimum in T in the main panel do not produce the same effect for a larger M (see the figure's inset). This behavior is well depicted in Figs. 3 and 4.

Figure 3 presents curves corresponding to the MFPT, T, as a function of the desorption rate δ, with $N = 20$, $\beta = 0.1$, for different system sizes in the y direction M. As can be seen from the figure, M significantly influences regime $\delta \gg 2\beta$. This is expected since there surface excursions are favorable and therefore are more dependent on the system size in the y direction. Notice that in regime $\delta \ll 2\beta$ (in particular, $\delta \ll \gamma$) all curves approach the same T; δ values in this regime, coupled with the initial distribution, prioritize paths on the baseline ($y = 0$), turning T insensitive to the values that M takes.

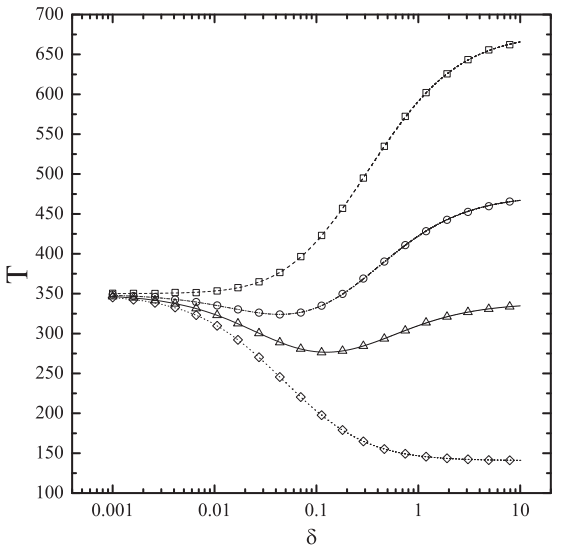

FIG. 3. MFPT as a function of the desorption rate (in log scale) δ, with $\beta = 0.1$, $N = 20$, for different values of M (system size in the y direction). From bottom to top $M = 4, 10, 14, 20$. Lines correspond to analytical calculations and symbols are for Monte Carlo simulations.

In Fig. 4 we draw the phase diagram that summarize the existence and nonexistence of enhanced transport analyzed from the perspective of the ocurrence of a minimum in the MFPT. The diagram is plotted for a fixed system size in the x direction $N = 20$ (inset: $N = 40$) as a function of the transition probability over the baseline β and the system size in the y direction M. White regions correspond to non-optimal transport (absence of minimum—monotonous behavior—in the MFPT), while darkened regions identify regimes with enhanced transport. We have also included in Fig. 4 curves

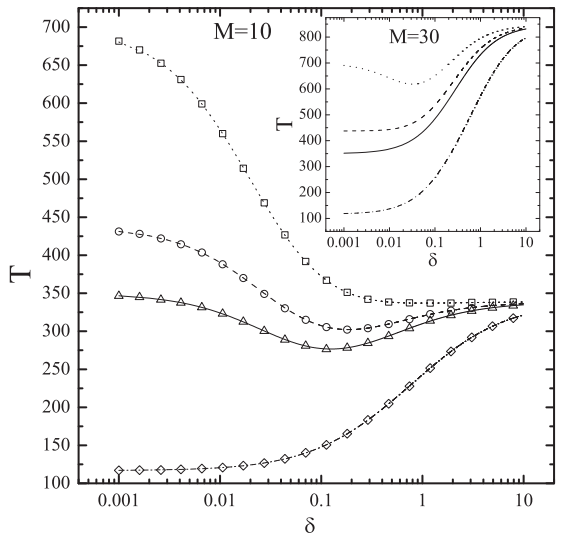

FIG. 2. MFPT as a function of the desorption rate (in log scale) δ, with $M = 10$ (inset: $M = 30$), $N = 20$, for different values of the transition rate (over the baseline) β. From bottom to top $\beta = 0.3, 0.1, 0.08, 0.05$. Lines correspond to analytical calculations and symbols are for Monte Carlo simulations.

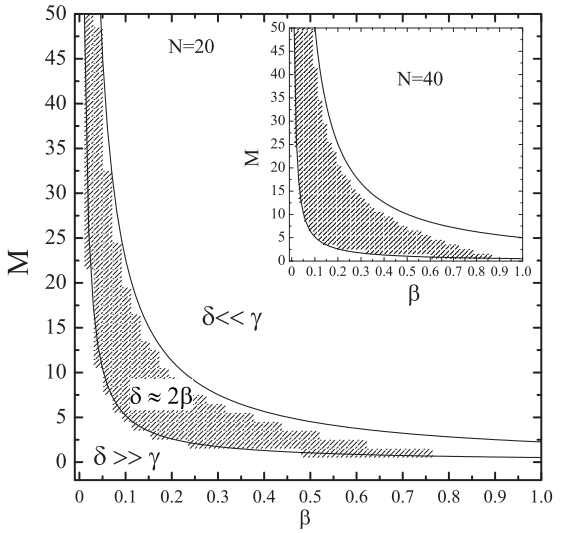

FIG. 4. Phase diagram that summarize the existence and nonexistence of enhanced transport, for a fixed system size in the x direction, N (Inset: $N = 40$.) White regions correspond to nonoptimal transport, while darkened regions identify regimes of enhanced transport. Lines correspond to the limit values of M determined by relation (19).

corresponding to the maximum of M, whose existence is a consequence of the transition from regime (i) to regime (ii), and to the minimum of M, caused by the transition from (ii) to (iii). These values are derived from Eq. (16),

$$\frac{1}{2\beta}\frac{a_2}{a_3-a_2} < \frac{M}{\gamma} < \frac{1}{2\beta}\left(\frac{a_1}{a_2}N-1\right); \tag{19}$$

a rough approximation ($a_1 \approx 0.16, a_2 \approx 0.6, a_3 \approx 1.18$) of (19) reads

$$\frac{N}{2\beta} < \frac{MN}{\gamma} < \frac{N^2}{2\beta}. \tag{20}$$

Let us take a closer look at the transition between regimes. To simplify our analysis we fix the values of β and N. Starting inside region $\delta \ll \gamma$ (this regime only involves 1D paths along the baseline) and decreasing M—δ starts to grow—$T \sim N^2/2\beta$ becomes similar to the overall time $NT_{\rm ret} = NM/\gamma + N/\delta$. This shows how an interplay between regimes (i) and (ii) begins, thus defining a maximum M. For values of M smaller than the maximum, a mixed type of transport [regime (ii)] prevails. This behavior remains until $NT_{\rm ret} = NM/\gamma + N/\delta$ becomes similar to $T \sim NM/\gamma$, defining a minimum M]transition from regime (ii) to (iii)]. There surface "journeys" dominate, and δ grows and approaches the limit $\delta \gg \gamma$. Notice that we obtain quite a good agreement between the region of optimal transport, evaluated from Eq. (14), and the corresponding bounds derived from relation (19).

IV. CONCLUSIONS

We have presented a simple model based on a master-equation approach to the narrow-escape-time problem. In this paper we introduced a type of confining domain that is alternative to the spherical one and we have considered the diffusion process on a lattice rather than in continuous space. Although the domain choice could have seemed arbitrary, we have shown that it fully reflects the behaviors of the general situation.

We have obtained analytic results for the basic quantity studied in the NET problem, the mean first-passage time (MFPT). We have also studied its dependence on the transition (desorption) probability over (from) the surface boundary, and the confining domain dimensions. In all cases the agreement between analytical results and Monte Carlo simulations was quite good.

We consider that the presented scheme is both simple enough to be studied analytically, and rich enough to mimic the impact of geometrical parameters in the system and the interplay between surface and boundary pathways. We believe that we have contributed to an area of growing interest which has motivated a great deal of work, giving a plausible physical insight into the surface-mediated diffusion mechanism. Thus, we have fulfilled our goal of presenting a simple model that captures in an unified framework the necessary ingredients to characterize the NET problem.

The present approach to the narrow-escape-time problem can be generalized in several directions: higher dimensions,"imperfect" detection, "dynamical" behavior of the narrow escape window, non-Markovian desorption, etc. All of these aspects will be the subject of future work.

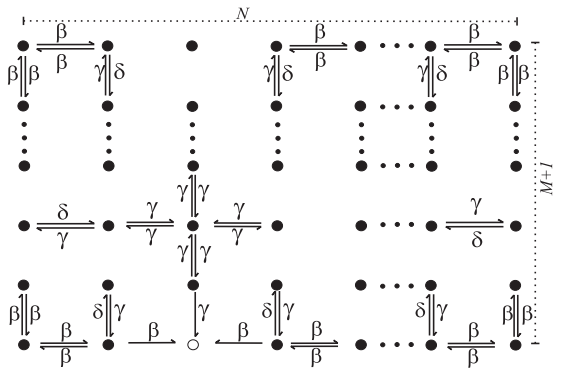

FIG. 5. Schematic transitions of the walker to or from the boundaries and to or from a generic surface site. Notice that the trap site (open circle) could be reached both from the surface (with transition rate γ) and from the baseline (with transition rate β).

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APPENDIX

In this Appendix we briefly discuss, through MC simulations, a more *general* confining domain, that is, when all the "walls" of the domain have δ as the desorption probability into the surface, and β as the transition probability over the boundaries (see Fig. 5). We keep γ as the surface transition probability per unit time in the x and y directions and we choose an uniform initial distribution over the boundaries for the walker.

The results given in Fig. 6 correspond to the MFPT as a function of the desorption rate δ for a fixed system size in x direction, $N = 20$. In Fig. 6(a) we have $M = 10$ and different values of the transition rate over the boundary,

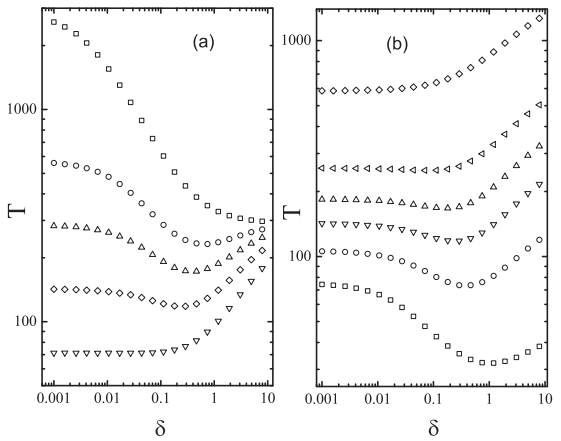

FIG. 6. (a) MFPT as a function of the desorption rate δ, with $M = 10$, $N = 20$, for different values of the transition rate (over the boundaries) β. From bottom to top $\beta = 0.1, 0.5, 1, 2, 4$. (b) MFPT as a function of δ, with $\beta = 2$, $N = 20$, for different values of M (system size in the y direction). From bottom to top $M = 2, 10, 14, 20, 40$. All results correspond to MC simulations.

β and in Fig. 6(b) we have $\beta = 2$ and different values of M (system size in the y direction). As can be seen from the figure, the original domain proposed (see Fig. 1) depicts a behavior similar to the general one. Notice the correspondence of the results of Fig. 6(a) with Fig. 2 and those from Fig. 6(b) with Fig. 3, respectively.

One may argue that, unlike Fig. 3, in Fig. 6(b) (as $\delta \to 0$) all curves approach a different T, however, this could be easily understood. For this situation the initial distribution is sensitive to the system size in the y direction M, since $g(n,m) = (1 - \delta_{n,0})\delta_{m,0}/(N-1) + \delta_{m,M}/N + (\delta_{n,0} + \delta_{n,N-1})/(M-1)$.

Besides the difference described above, our original model (Fig. 1) qualitatively reflects the behaviors of the general (Fig. 5) one, thus enabling us to extract reliable information of a complex-general situation through the analysis of our simpler, original scheme.

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