I. INTRODUCTION

The time needed for a particle contained in a confining domain with a single small opening to exit the domain for the first time, usually referred as narrow escape time problem (NET), finds a prominent place in many domains and fields. For instance in cellular biology, it is related to the random time needed by a particle released inside a cell to activate a given mechanism on the cell membrane ([1–3]). Generally speaking the NET problem is part of the so called Intermittent processes, which are used to explain scenarios ranging from animal search patterns ([4]), through the solutions or melts of synthetic macromolecules ([5, 6]), to the manufacture of self-assembled mono- and multi-layers ([7, 8]). Since the problem of return to the system, i.e. once the particle reaches the domain for the first time. We introduce a finite transition probability, ν, at the narrow escape window allowing the study of the imperfect trapping case. Ranging from 0 to ∞, ν allowed the study of both extremes of the trapping process: that of a highly deficient capture, and situations where escape is certain (“perfect trapping” case). We have obtained analytic results for the basic quantity studied in the NET problem, the mean escape time (MET), and we have studied its dependence in terms of the transition (desorption) probability over (from) the surface boundary, the confining domain dimensions, and the finite transition probability at the escape window. Particularly we show that the existence of a global minimum in the NET depends on the ‘imperfection’ of the trapping process. 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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II. ANALYTICAL APPROACH

A. Some general results regarding imperfect trapping

Let us consider the problem of a walker making a random walk in some finite domain with a trap or sink present in the system. We will follow the walker evolution through the system considering the ‘unrestricted’
conditional probability $P(\vec{s},t|\vec{s}_0,t = 0)$, that is, the probability that a walker is at $\vec{s}$ at time $t$ given it was at $\vec{s}_0$ at $t = 0$. By ‘unrestricted’ we identify a situation with no traps/sinks present in the system.

FIG. 1. Finite domain with a trap or sink present. The entrance to the trap site (empty circle) is regulated at the escape ‘window’ by the transition rate $\nu$.

Absorption Probability Density and Mean Absorption Time

As we are interested in the trapping process, let us define $A(\vec{s},t|\vec{s}_0,0)$ as the Absorption (trapping) Probability Density (APD) through the site $\vec{s}$ at time $t$, given that the walker was at $\vec{s}_0$ at time $t = 0$, i.e., $A(\vec{s},t|\vec{s}_0,0)\, dt$ gives the trapping probability of the walker, through $\vec{s}$, between $t$ and $t + dt$ given that it started at $t = 0$ from $\vec{s}_0$. It is worth mentioning that the First Passage time approach is not fully applicable since an ‘excursion’ to the trapping site does not necessarily ends the process. However we show in the following lines that an interesting relation could be established between $A(\vec{s},t|\vec{s}_0,0)$ and $F(\vec{s},t|\vec{s}_0,0)$, the First Passage time density (FPTD) through the site $\vec{s}$ at time $t$, given that the walker was at $\vec{s}_0$ at time $t = 0$.

From now on we will denote the Laplace transform of a function $f(t)$ by its argument,

$$\mathcal{L}\{f(t)\} = f(u) = \int_0^\infty e^{-ut}f(t)\, dt.$$ 

The connection between the APD and the ‘unrestricted’ conditional probability $P(\vec{s},t|\vec{s}_0,t = 0)$ could be traced to results in [23] or [27]. This approach in the Laplace domain gives,

$$A(\vec{0}, u|\vec{s}_0, t = 0) = \frac{\nu P(\vec{0}, u|\vec{s}_0, t = 0)}{1 + \nu P(0, u|0, t = 0)}.$$ (1)

Let us make a brief digression regarding the relation between the APD and the FPTD. For this we rewrite Eq. (1) in the form

$$A(\vec{0}, u|\vec{s}_0, t = 0) = \frac{P(\vec{0}, u|\vec{s}_0, t = 0)}{P(0, u|0, t = 0)} \cdot \frac{\nu}{1 + \nu}$$ (2)

As usual the connection between FPTD and the ‘unrestricted’ conditional probability $P(\vec{s},t|\vec{s}_0, t = 0)$ is established (in the Laplace domain) through the ‘Renewal approach’ (28).

$$F(\vec{0}, u|\vec{s}_0, t = 0) = \frac{P(\vec{0}, u|\vec{s}_0, t = 0)}{P(\vec{0}, u|0, t = 0)}.$$ (3)

We recognize in equation (2), the FPTD (3) and using the relation $F(\vec{0}, u|0, t = 0) = 1 - \Psi(\vec{0}, u)P(0, u|0, t = 0)$

where $\Psi(\vec{s}, t)$ is the probability that the walker remains at $\vec{s}$ until time $\tau$ since it arrived at $\vec{s}$ at time 0 (in the unrestricted case) [29], we rewrite Eq. 2 as

$$A(\vec{0}, u|\vec{s}_0, t = 0) = F(\vec{0}, u|\vec{s}_0, t = 0)$$

$$\frac{\nu}{1 + \nu} \cdot \frac{1}{1 - \Psi(\vec{0}, u)^{-1}} F(\vec{0}, u|0, t = 0)$$ (4)

The term $\nu(\Psi(\vec{0}, u)^{-1} + \nu)^{-1}$ in [31] gives the fraction of walkers that are trapped while $\Psi(\vec{0}, u)(\Psi(\vec{0}, u)^{-1} + \nu)^{-1}$ gives the ones that are not absorbed. Further considerations could be made regarding [41], we write it as,

$$A(\vec{0}, u|\vec{s}_0, t = 0) = \sum_{j=1}^{\infty} A_j(\vec{0}, u|\vec{s}_0, t = 0),$$ (5)

where

$$A_j(\vec{0}, u|\vec{s}_0, 0) = F(\vec{0}, u|\vec{s}_0, 0)\left(\frac{F(\vec{0}, u|0, 0)\Psi(\vec{0}, u)^{-1}}{\Psi(\vec{0}, u)^{-1} + \nu}\right)^{j-1} \cdot \frac{\nu}{\Psi(\vec{0}, u)^{-1} + \nu}.$$ (6)

Notice that $A_j(\cdot)$ accounts for that walkers that are absorbed in the $j$-visit ($j = 2,3,\ldots$) and not before, i.e., the walkers arrive for the first time at site $\vec{0}$ from $\vec{s}_0$ but these are not absorbed until they return to site $\vec{0}$ for the $(j-1)$-time.

The probability of being absorbed in the $j$-visit at site $\vec{0}$ is,

$$\int_0^\infty A_j(\vec{0}, t|\vec{s}_0, 0)\, dt = A_j(\vec{0}, u = 0|\vec{s}_0, 0) = \left(\frac{\Psi(\vec{0}, 0)^{-1}}{\Psi(\vec{0}, 0)^{-1} + \nu}\right)^{j-1} \left(\frac{\nu}{\Psi(\vec{0}, 0)^{-1} + \nu}\right),$$ (7)

where $\Psi(\vec{0}, u) = 0$ is the mean residence time at site $\vec{0}$ in the unrestricted system and we have used that $F(\vec{s}, u = 0|\vec{s}_0, t = 0) = 1$ for a finite (unrestricted) system. As equation (7) shows, when $\nu \to 0$ independently of the $j$ value, we have no absorption, while in the limit $\nu \to \infty$ the absorption is certain in the first ‘visit’ to the site (i.e. $j = 1$).

The mean absorption time, i.e., the mean time until the walker is absorbed is evaluated in terms of $A(\cdot)$ as,

$$T = \int_0^\infty t \sum_{\vec{s}_0} A(\vec{0}, t|\vec{s}_0, 0)g(\vec{s}_0)\, dt$$

$$= -\frac{\partial}{\partial u} \left\{ \sum_{\vec{s}_0} A(\vec{0}, u|\vec{s}_0, 0)g(\vec{s}_0) \right\} \bigg|_{u=0}$$ (8)
where \( q(\vec{s}_0) \) denotes the probability density of initially finding the walker at a position \( \vec{s}_0 \) \( (28) \).

**B. The Model**

For our model we consider the problem of a walker making a random walk in a finite rectangular \( N \times (M+1) \) lattice (see figure 2). 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. As we mentioned before, we follow the walker’s evolution through the system considering the conditional probability \( P(n, m, t|n_0, m_0, t = 0) \equiv P(n, m, t) \), where \( (n, m) \) are discrete coordinates in the \( (x, y) \) space. \( P(n, m, t) \) satisfies the following master equation:

\[
\begin{align*}
\dot{P}(n, 0, t) &= \gamma P(n, 1, t) - \delta P(n, 0, t) \\
&+ \beta (P(n + 1, 0, t) + P(n - 1, 0, t)) \\
&- 2P(n, 0, t); \quad m = 0 \\
\dot{P}(n, 1, t) &= \delta P(n, 0, t) - 4\gamma P(n, 1, t) \\
&+ \gamma (P(n + 1, 1, t) + P(n - 1, 1, t)) \\
&+ P(n, 2, t); \quad m = 1 \\
\dot{P}(n, m, t) &= \gamma (P(n - 1, m, t) + P(n + 1, m, t) \\
&+ P(n, m + 1, t) + P(n, m - 1, t)) \\
&- 4\gamma P(n, m, t); \quad 2 \leq m \leq M - 1 \\
\dot{P}(n, M, t) &= \gamma (P(n - 1, M, t) + P(n, M + 1, t) \\
&+ P(n, M - 1, t)) \\
&- 3\gamma P(n, M, t); \quad m = M
\end{align*}
\]

(9)

where \( \gamma \) is the surface transition probability per unit time in the \( x \) and \( y \) direction, \( \beta \) is the transition probability over the line \( m = 0 \) in the \( x \) direction, and \( \delta \) is the desorption probability per unit time from the boundary line \( m = 0 \).

We introduce the imperfect escape case by allowing a finite transition probability (\( \nu \)) at the narrow escape window. Varying from 0 to \( \infty \), \( \nu \) allowed the study of both a deficient trapping, and situations where escape is certain (i.e. perfect trapping case).

In the following we will say that the walker ‘escapes’ when it gets trapped or adsorbed, without the possibility of returning to the system. This terminology matches the one used in the NET area. Hence, \( \text{adsorption} \rightarrow \text{escape} \), and so on.

**Escape Probability Density (EPD)**

We now make a brief comment regarding the Escape Probability Density. Taking into account the parameters of our model, we could write equation (11) as,

\[
\int_0^\infty A_j(\tilde{\theta}, t|\tilde{s}_0, 0)dt = A_j(\tilde{\theta}, u = 0|\tilde{s}_0, 0) = \left(\frac{2\beta + \delta}{2\beta + \delta + \nu}\right)^{j-1}\left(\frac{\nu}{2\beta + \delta + \nu}\right).
\]

Notice that as \( \nu \) grows (\( \nu >> 2\beta + \delta \)) each \( A_j \) becomes smaller except for \( A_1 \), with \( A_1 \rightarrow 1 \), i.e. the escape is certain in the first visit. However when \( \nu << 2\beta + \delta \), the probability of escape \( A_j(\cdot) \) has contributions from each \( j \)-visit. This can best be understood considering,

\[
\frac{A_j(\cdot)}{A_{j+1}(\cdot)} \bigg|_{u=0} = 1 + \frac{\nu}{2\beta + \delta} \quad (j \neq 1)
\]

(11)

which gives the relative contribution of successive terms in (5). When \( \nu \) gets smaller the contribution is spread all over \( j \)-values as Eq. (11) shows. In contrast, each \( A_j \rightarrow 0 \) (\( j \neq 1 \)) as \( \nu \) grows, concentrating all the probability in \( A_1 \).

**Mean Escape Time (MET)**

Following the ideas exposed in [19] and by resorting to the matrix formalism and the Dyson’s procedure (26) we were able to obtain the probability \( P(n, m, t|n_0, m_0, t = 0) \) (in the Fourier-Laplace space), which is the building block for the MET. For the detailed calculation see appendix [A].

We will denote the (finite) Fourier transform by its argument, as we did in the Laplace transform case. Thus
For example the transform on a coordinate, say $x$, would read:
\[
P(k,m,t\mid n_0,m_0,0) = \mathcal{F}\{P(n,m,t\mid n_0,m_0,0)\} = \sum_{n=0}^{N-1} e^{i kn} P(n,m,t\mid n_0,m_0,0).
\]
From $P(k,m,u\mid n_0,m_0,t = 0)$ (obtained in the Fourier-Laplace space), 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 $t = 0$, $P(n,m,t\mid n_0,m_0,0)$, is derived by using the inverse Laplace transform on $u$ and the inverse Fourier transform on $k$ (for the $x$ coordinate) for each $[\mathbb{P}(k,u)]_{n_0,m_0}$. However, as we are interested in the calculation of $\mathbb{M}$, we only need to perform the inverse Fourier transform on $P(0,0,u\mid n_0,m_0,t = 0)$, i.e. we need the elements $\mathcal{F}^{-1}\{[\mathbb{P}(k,u)]_{0,m_0}\}$. We obtain for $[\mathbb{P}(k,u)]_{0,m_0}$:
\[
[\mathbb{P}(k,u)]_{0,m_0} = \frac{\eta_{m_0}^{\delta^*} + \eta_{M-m_0}^{\delta^*}}{\delta (1 - \eta)(1 - \eta^{-M}) + (u - A_1(k))(1 + \eta^{M})},
\]
where $\eta = 1 + (\bar{u} - \sqrt{\bar{u}^2 + 4 \gamma \bar{u}})/2 \gamma$, $M = 2M + 1$ and $\bar{u} = u - A_1(k)$. The inverse Fourier transform on $[\mathbb{P}(k,u)]_{0,m_0}$ is carried out in the following way,
\[
P(0,0,u\mid n_0,m_0,0) = \frac{1}{N} \sum_{q=0}^{N-1} e^{i 2\pi \delta q} [\mathbb{P}(\frac{2\pi q}{N}, u)]_{0,m_0} \tag{13}
\]
Thus we have obtained the required expression for the calculation of the MET through the narrow escape window and it only remains to choose the initial distribution. We now evaluate the MET for a walker with an uniform initial distribution on the base line ($y = 0$). This means the initial distribution is given by $g(n,m) = (1 - \delta_{n_0})\delta_{m_0}/(N-1)$. Notice that we explicitly exclude the possibility of having a walker at $(0,0)$ at $t = 0$ \cite{note}. This way we obtain,
\[
T = N \left[ \frac{M + 1}{\gamma} + \sum_{q=0}^{N-1} \left[ \frac{\mathbb{P}(\frac{2\pi q}{N}, u = 0)}{N - 1} \right]_{0,0} \right] \tag{14}
\]
We make some comments regarding equation (13) which constitutes one of our main results. Notice that (14) adequately provides the limits of perfect escape case, $\nu \to \infty$ (obtained in (13)) and no escape window, $\nu \to 0$, $T \to \infty$. Observe that as it is commented in (10) for a perfect escape case, $T$ could be expressed in the following way,
\[
T = \frac{NM}{\gamma} \left[ \frac{\delta}{\nu} + \sum_{q=0}^{N-1} \left[ \frac{\mathbb{P}(\frac{2\pi q}{N}, u = 0)}{N - 1} \right]_{0,0} \right] + \frac{N}{2\beta} \left[ \frac{2\beta}{\nu} + 2\beta \sum_{q=0}^{N-1} \left[ \frac{\mathbb{P}(\frac{2\pi q}{N}, u = 0)}{N - 1} \right]_{0,0} \right] \tag{15}
\]
or $T = T_{\text{surface}} + T_{\text{line}}$; \cite{note} provides an interesting physical insight into the problem. Simply notice how the mean escape time is constructed from the mean duration of surface excursions and the mean duration of border or line excursions (first and second terms of (15) respectively).

Regarding the existence of a minimum in $T$

$T$ could be enhanced with respect to $\delta$ provided we are able to find $\delta^* = \delta^*(\beta, \gamma, \nu, N, M)$ - the optimal desorption probability - that satisfies,
\[
\frac{\partial T}{\partial \delta} \bigg|_{\delta = \delta^*} = \frac{NM}{\gamma \nu} + \sum_{q=0}^{N-1} \sum_{i=0}^{\infty} \left[ \frac{2\alpha_1^i M^{-1} 2\beta \alpha_2 - \alpha_1}{(\alpha_1 \delta^* + \alpha_2 \beta)^2} \right] = 0 \tag{16}
\]
where the $\alpha_i = \alpha_i(q, N, M)$ for $i = 1, 2$ are defined in appendix (13). Notice that (16) defines an implicit equation for $\delta^*$ which, although we could not solve, provided us with some generals conclusions as it approaches certain limits. Consider first $\beta \to 0$, with the other parameters held fixed. In this case (a finite value for $\delta^*$) exists whenever we have a finite escape probability rate $\nu$ and,
\[
\delta^* = \sqrt{\frac{\nu \gamma}{M(N-1) \sum_{q=0}^{N-1} \alpha_1^i}}. \tag{17}
\]
This is a highly interesting result since in the perfect escape case ($\nu = \infty$) this minimum disappears, as $\delta^*$ is pushed towards $\infty$. Thus the ‘imperfect’ escape window enables a region that was absent in the perfect case. On the other hand in the limit $\beta \gg \delta$ it could be shown that equation (16) can not be satisfied for any $\delta^*$ value. 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.

In the following section we will make more remarks regarding the minimum in $T$, while introducing some implications corresponding to $\delta^*$. 

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 while symbols correspond to Monte Carlo (MC) simulations. We will be interested in situations in which a mixed type of transport generates a global minimum in the Mean Escape Time.

In Fig. 3 we present curves corresponding to the MET (Mean Escape Time), as a function of the desorption rate $\delta$, with parameters $N = 20$, $M = 10$ and $\beta = 0.1$, for different values of the escape ‘strength’ $\nu$, which is the ‘transition rate’ at the escape window. We have included for comparison the ‘perfect escape case’, i.e. once in the escape window the escape is instantaneous, with no
for this situation we could say that rises the T curve until it becomes monotonous. Hence, the transition rate at the escape window can contribute positively as well. This behavior is well depicted in figure 4.

Figure 3 presents curves corresponding to the Mean Escape Time, as a function of the desorption rate $\delta$, with $N = 10$, $M = 2$, $\beta = 0.01$, for different values of the transition rate $\nu$. As can be inferred from the figure, $\nu$ significantly influences MET as it varies from 0 to $\infty$. Changes in the location of the extrema values of MET can be seen ranging from a monotonous behavior ($\nu \to \infty$ extrema in $\delta \to \infty$) to a situation with a global minimum, and then back again into a monotonous behavior ($\nu \to 0$ extrema in $\delta \to 0$). So in this case the transition rate to the escape window contributes 'positively' to the mixed type of transport, since it turns a situation without a minimum (perfect escape case) into a situation of enhanced transport (minimum in T for some values of $\nu$).

In Fig. 3 we present curves corresponding to the $\delta$ value that minimizes MET, $\delta^*$, as a function of $\beta$ for different values of $\nu$, obtained from the numerical solution of Eq. (10). All lines depict quite a similar trend for finite $\nu$; $\delta^*(\beta, N, M, \gamma, \nu) = 0$ values marked by empty circles are not included in the curves and mark the end of the $\beta$-interval in which $\delta^*$ exists. In other words $T$ is not monotonous while $\beta \in [0, \beta_0]$. As we show in Appendix $\beta_0$ satisfies,

$$2\beta_0 = \frac{\gamma}{M} \frac{\sum_{q=1}^{N-1} \alpha_1 \alpha_2^{-2}}{\sum_{q=1}^{N-1} \alpha_1^{-2}}$$

(18)

For values larger than $\beta_0$ the T curve reaches a minimum at $\delta = 0$. However this is found at the beginning of the $\delta$-interval and without change of sign of $\partial T/\partial \delta$. We decided to rule it out as long as it doesn’t represent a true interplay between surface and boundary paths. In these situations all particles stay in the base line and eventually escape through the escape window without excursions into the surface.

The behavior of $\delta^*$ considerably changes in the perfect case ($\nu = \infty$). Particularly the range of $\beta$ values where a minimum exists in T shrinks as indicated by the dashed asymptotes in the figure. The left/right asymptotes indicate the limit in which T becomes monotonous, extrema for $\delta^* \to \infty$ and $\delta^* \to 0$ respectively. The left and right asymptotes are respectively located at,

$$2\beta_{\delta^* \to \infty} = \frac{\gamma}{M} \sum_{q=1}^{N-1} \alpha_1^{-1} \left( \sum_{q=1}^{N-1} \alpha_2 \alpha_1^{-2} \right)^{-1}$$

(19)

$$2\beta_{\delta^* \to 0} = \frac{\gamma}{M} \sum_{q=1}^{N-1} \alpha_1 \alpha_2^{-2} \left( \sum_{q=1}^{N-1} \alpha_1^{-1} \right)^{-1}$$

(20)
For clarity’s sake in the inset we have magnified the entry points to the \( \beta \) axis of \( \delta^* \) curves for \( \nu = 10, 100, \infty \).

Figure 6 shows the phase diagrams that summarize the existence/non-existence of enhanced transport, analyzed from the perspective of the existence of a minimum in the Mean Escape Time. The diagrams are plotted for fixed \( N, M \) and \( \nu \) as a function of the transition probability over the baseline, \( \beta \), and the surface transition probability \( \gamma \). White regions correspond to non-optimal transport (absence of minimum -monotonic behaviour- in the MET), while filled regions (red patterns) identify regimes of enhanced transport. Region enclosed by black lines correspond to enhanced transport in the perfect trapping case \((\nu = \infty)\) while dashed (green) lines correspond to the bound -from eq. 18- after which, \( T \) becomes monotonous.

and [19], [20] for \( \nu = \infty \).

IV. CONCLUSIONS

We have presented a model based on a master equation approach to the narrow escape time problem. In this study we introduced a finite transition probability, \( \nu \), at the narrow escape window which allowed us to study the imperfect escape case. Varying from 0 to \( \infty \), \( \nu \) allowed the study of both extremes of the trapping process: that of a highly deficient capture, and situations where escape is certain (perfect trapping case).

By resorting to Dyson technique we have obtained analytic results for the primary quantity studied in the NET problem, the Mean Escape Time (MET), and we have studied its dependence in terms of the transition (desorption) probability over (from) the surface boundary, the confining domain dimensions, and the finite transition probability at the escape window. Particularly we showed that the existence of a global minimum in the NET is controlled by the ‘imperfection’ of the escape process. Regarding such conclusion, a very interesting result was that the ‘imperfect’ escape window enabled a region
where $T$ could be minimized, something the perfect case lacked.

We have also presented bounds -equations (18), (19) and (20)- between which an optimal minimum value of $T$ could be found, improving previous bounds derived in (19). The phase diagrams introduced in the last section deserve a special word, for not only do they present a compact summary of the situations of enhanced transport, whenever some exist, but they also can lead to a better understanding of the relations among the parameters that characterize the system. In addition to our analytical approach, we have implemented Monte Carlo simulations, finding excellent agreement between the theoretical results and simulations.

We consider that the presented scheme is an analytically manageable model, which could be used to study the impact of several (domain dimension, different rates of transition, etc.) parameters in the interplay between surface and boundary pathways, and could also serve as a forerunner for the study of more general and complex systems. This work contributes to an area of growing interest, providing a more general overview of a previous work (19) and showing a plausible physical insight into the surface-mediated diffusion mechanisms in the presence of an imperfect escape window.

The current approach to the narrow escape time problem can be generalized in several directions: higher dimensions, “dynamical” behaviour of the narrow escape window, non-markovian desorption, etc. All of these aspects will be the subject of future work.

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Appendix A: MET calculation

In this appendix we focus on the calculation of the probability $P(n,m,t|n_0,m_0,t=0)$, which is the building block for the Mean Escape Time. Taking the (finite) Fourier transform with respect to the $x$ variable and the Laplace transform with respect to the time $t$ in Equation (9), we obtain:

$$uP(k,0,u) − P(k,0,t = 0) = \gamma P(k,1,u) − (\delta − A_1(k))P(k,0,u)$$

$$m = 1$$

$$uP(k,1,u) − P(k,1,t = 0) = \delta P(k,0,u) + \gamma P(k,2,u) − (2\gamma − A(k))P(k,1,u)$$

$$2 \leq m \leq M − 1$$

$$uP(k,m,u) − P(k,m,t = 0) = A(k)P(k,m,u) + \gamma (P(k,m+1,u) + P(k,m−1,u)) − 2\gamma P(k,m,u)$$

$$m = M$$

$$uP(k,M,u) − P(k,M,t = 0) = A(k)P(k,M,u) + \gamma P(k,M−1,u) − \gamma P(k,M,u).$$

(A1)

Here we have defined $A_1(k) = 2\beta(\cos k − 1)$, $A(k) = 2\gamma(\cos k − 1)$. Using the matrix formalism, equation (A1) can be written as

$$[uI − \mathbb{H}]P = \mathbb{I},$$

(A2)

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

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

(A3)

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

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

In order to find the solution to equation (A2) we decompose the $\mathbb{H}$ matrix in the following way,

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

(A4)

where

$$\mathbb{H}^0 = 
\begin{bmatrix}
−\gamma & \gamma & 0 & \ldots & 0 \\
\gamma & −2\gamma & \gamma & 0 & \ldots \\
0 & \gamma & −2\gamma & \gamma & 0 \\
\ldots & \ldots & \gamma & −2\gamma & \gamma \\
\ldots & \ldots & 0 & \gamma & −\gamma
\end{bmatrix},$$

(A5)

corresponds to the transition matrix for a symmetric random walk to nearest neighbours in a finite lattice ($M+1$...
\[ \mathbb{H}^1 = (\gamma - \delta + A_1(k) - A(k))\delta_{i,0}\delta_{0,j} = \Delta_1\delta_{i,0}\delta_{0,j} \quad (A6) \]

\[ \mathbb{H}^2 = -(\gamma - \delta)\delta_{i,1}\delta_{0,j} = \Delta_2\delta_{i,1}\delta_{0,j} \quad (A7) \]

A formal solution to equation (A2) is:

\[ \mathbb{P} = [u\mathbb{I} - \mathbb{H}]^{-1}. \quad (A8) \]

By applying the Dyson procedure (20) a general expression in the Fourier-Laplace space for \( [\mathbb{P}(k, u)]_{m, m_0} \) could be found,

\[ [\mathbb{P}(k, u)]_{m, m_0} = [\mathbb{P}^0(k, u)]_{m, m_0} + [\mathbb{P}^0(k, u)]_{m, 0} \cdot \frac{\Delta_1}{1 - \Delta_1 [\mathbb{P}^0(k, u)]_{0, 0}} \cdot \frac{\Delta_1}{1 - \Delta_1 [\mathbb{P}^0(k, u)]_{0, 0}} \cdot \left( [\mathbb{P}^0(k, u)]_{m, 1} + \frac{\Delta_1}{1 - \Delta_1 [\mathbb{P}^0(k, u)]_{0, 0}} \right) \quad (A9) \]

where,

\[ [\mathbb{P}^0(k, u)]_{m, m_0} = \eta^{m-m_0} + \eta^{M-(m+m_0)} \]

\[ \hat{u} = u - A(k), \quad \hat{M} = 2M + 1 \quad \text{and} \quad \eta = 1 + \left( \hat{u} - \sqrt{\hat{u}^2 + 4\gamma^2} \right) / 2\gamma. \]

From (A9), the probability that a walker is 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 \(x\) coordinate for each matrix element \([\mathbb{P}(k, u)]_{m, m_0}\). Notice that, as we are interested in the calculation of \(S\), 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 \(F^{-1}\{[\mathbb{P}(k, u)]_{0, m_0}\}\). In this case expression (A9) reduces to,

\[ [\mathbb{P}(k, u)]_{0, m_0} = \eta^{m_0} + \eta^{M_{-m_0}} \]

\[ \delta(1-\eta)(1-\eta^{M+1}) + (u - A(k))(1 + \eta^{M}) \quad (A10) \]

The inverse Fourier transform on \([\mathbb{P}(k, u)]_{0, m_0}\) is carried out in the following way,

\[ P(0, 0, u | n_0, m_0, t = 0) = \frac{1}{N} \sum_{q=0}^{N-1} e^{i2\pi\eta/N} [\mathbb{P}(2\pi q/N, u)]_{0, m_0}. \quad (A11) \]

Thus we have obtained all the required expressions for the calculation of the MET. We now proceed to evaluate the Mean Escape Time for a walker with an uniform initial distribution on the base line \((y = 0)\), i.e. \(g(n, m) = (1 - \delta_{m,0})\delta_{m,0}/(N - 1)\). Notice that we explicitly exclude the possibility of having a walker at \((0, 0)\) at \(t = 0\). We obtain,

\[ T = N \left[ \frac{M}{\gamma} + \frac{1}{\delta} \right] \left\{ \frac{\delta}{\nu} + \frac{\delta}{N-1} \sum_{q=1}^{N-1} \left[ \mathbb{P}(2\pi q/N, u = 0) \right]_{0, 0} \right\} \quad (A12) \]

Appendix B: \( \delta^* \) - optimal desorption probability

In this section we present some results regarding the desorption probability rate value that minimizes \(T, \delta^*\). For this recall equation (16),

\[ \frac{\partial T}{\partial \delta} |_{\delta = \delta^*} = \frac{N M(1 - \eta u_0)(1 - \eta q M)}{\gamma N} + \frac{N - 1}{N} \sum_{q=1}^{N} M \gamma^{-1} 2\beta \omega_2 - \alpha_1 (\alpha_1 \delta^* + \alpha_2 2\beta)^2 = 0 \quad (B1) \]

Let us focus on the relation between \(\delta\) and \(\beta\) as these are the parameters of interest, since the former enables the transport on the surface, and the later regulates the movement on the boundary line where the escape window is located. Although we will keep track of all variables, it could be shown that (B1) can be written in terms of the scaled variables \(\beta' = \beta \gamma^{-1}, \quad \nu' = \nu \gamma^{-1}\) and \(\delta' = \delta \gamma^{-1}\). So a modification in \(\gamma\) would result in an enlargement or shrinkage (if we let \(\delta' = 0\)). Notice that we explicitly exclude the possibility of having a walker at \((0, 0)\) at \(t = 0\). We obtain,

\[ T = N \left[ \frac{M}{\gamma} + \frac{1}{\delta} \right] \left\{ \frac{\delta}{\nu} + \frac{\delta}{N-1} \sum_{q=1}^{N-1} \left[ \mathbb{P}(2\pi q/N, u = 0) \right]_{0, 0} \right\} \quad (A12) \]
Then after some algebra we obtain,
\[
\frac{\partial \delta^*}{\partial \beta} = \sum_{q=1}^{N-1} \frac{M_{\gamma-1} \alpha_q \alpha_2}{\sum_{q=1}^{N-1} M_{\gamma-1} \alpha_q} - \sum_{q=1}^{N-1} \frac{M_{\gamma-1} \alpha_2}{\sum_{q=1}^{N-1} M_{\gamma-1} \alpha_q} \tag{B2}
\]
From (B2) we could obtain the entry points to the \( \beta \) axis of \( \delta^* \) curves. The forerunner for this is the sharp growth on the \( \delta^* \) curves in figure (4). As a matter of fact the abrupt increase is in \( \partial \log \delta^*/\partial \log \beta \). However is not difficult to show that this happens only if the denominator in \( \delta^* \rightarrow 0 \) for some \( \beta_0 \) (also notice that in this situation \( \delta^* \sim 0 \) so,
\[
\sum_{q=1}^{N-1} \frac{\alpha^2}{(\alpha_2 \beta_0)^2} = M_{\gamma-1} \sum_{q=1}^{N-1} \frac{\alpha^2}{(\alpha_2 \beta_0)} \tag{B3}
\]
where we have used \( \text{(B1)} \) to replace the sum on the right hand side. We could go even further and replace the sum on the left hand side. For this we differentiate \( \text{(B1)} \) with respect to \( \delta^* \) and get \( M_{\gamma-1} \frac{\alpha}{\partial_2 \beta_0} = \frac{2}{(N-1)} + 2 \beta_0 \sum_{q=1}^{N-1} \frac{\alpha^2}{(\alpha_2 \beta_0)^2} \). By using this relation and rearranging some terms in \( \text{(B3)} \) we finally obtain,
\[
2 \beta_0 = \frac{\gamma}{M} \sum_{q=1}^{N-1} \alpha^2 - \frac{1}{\sum_{q=1}^{N-1} \alpha^2} \tag{B4}
\]
The solution of equation \( \text{(B4)} \) in terms of \( \beta_0 \) that makes \( \delta^*(\beta_0, N, M, \gamma, \nu) = 0 \) marks the end of the interval in which \( \delta^* \) exists i.e., the T curve becomes monotonous.

For the perfect escape case we obtain one of the asymptotes between which \( \delta^* \) exits, outside them the extrema is pushed either to 0 or to \( \infty \), by letting \( \nu \rightarrow \infty \) in \( \text{(B4)} \),
\[
2 \beta_0 \rightarrow 0 = \frac{\gamma}{M} \sum_{q=1}^{N-1} \alpha^2
\]
For the second asymptote we go back to \( \text{(B2)} \), follow a similar reasoning that lead us to equation \( \text{(B3)} \), here \( \nu = \infty \), \( \delta^* \rightarrow \infty \), and obtain,
\[
2 \beta_0 \rightarrow \infty = \frac{\gamma}{M} \sum_{q=1}^{N-1} \alpha^2
\]
Equations \( \text{(B5)} \) and \( \text{(B6)} \) constitute an improvement to the bounds derived in \( \text{[19]} \) and the solution of equation \( \text{(B4)} \) gives an improvement to the literature known by us regarding the existence of a minimum in the MET.

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[29] See [22] and references therein.

[30] This consideration will help us in the comparison with the perfect escape case and avoids the ‘instantaneous’ escaping in the limit $\nu \to \infty$. 