Trapping of particles diffusing in two dimensions by a hidden binding site

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We study trapping of particles diffusing in a two-dimensional rectangular chamber by a binding site located at the end of a rectangular sleeve. To reach the site a particle first has to enter the sleeve. After that it has two options: to come back to the chamber or to diffuse to the site where it is trapped. The main result of the present work is a simple expression for the mean particle lifetime as a function of its starting position and geometric parameters of the system. This expression is obtained by an approximate reduction of the initial two-dimensional problem to the effective one-dimensional one which can be solved with relative ease. Our analytical predictions are tested against the results obtained from Brownian dynamics simulations. The test shows excellent agreement between the two for a wide range of the geometric parameters of the system.

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I. INTRODUCTION

This paper presents a theoretical study of trapping of diffusing particles by a hidden binding site in two dimensions in the geometry shown in Fig. 1(a), which is a special case of diffusion-limited reactions. Theoretical investigations of such processes were initiated by Smoluchowski [1], who considered trapping of diffusing particles by a perfectly absorbing immobile sphere [2,3]. Further development of the theory involved generalization of the Smoluchowski analysis in different directions. One of them is trapping by nonuniform surfaces pioneered by Hill [4] and Berg and Purcell [5]. In their analysis, to be trapped, a diffusing particle has to find an absorbing patch on the otherwise reflecting surface. A more complicated problem arises when a binding site is hidden in a tunnel. In this case, a particle first has to find an entrance to the tunnel leading to the site. Entering the tunnel, the particle either diffuses to the binding site, where it is trapped, or escapes from the tunnel back to the bulk solution. Studies of this notoriously complicated problem in three dimensions were initiated by Samson and Deutch [6]. Their work was generalized by Zhou [7] who used the constant flux approximation proposed by Szabo and coauthors [8]. Later this problem was analyzed in Refs. [9,10], where the constant flux approximation was abandoned.

Here, we study a two-dimensional version of the problem in the geometry shown in Fig. 1(a). Specifically, we consider a point particle diffusing in a rectangular chamber of length L and width W, which, at the center of its right wall, has a sleeve of length l and width $w \leqslant W$ terminated by a binding site, where the particle is trapped as soon as it touches the site for the first time. The quantity of our interest is the mean lifetime of a particle starting in the chamber, denoted by $\tau_l(x_0)$, where x_0 is the distance of the particle starting point from the chamber wall opposite to the side containing the sleeve entrance [see Fig. 1(a)]. We derive a simple approximate expression giving $\tau_l(x_0)$ as a function of the geometric parameters L, W, l, w, and x_0,

$$\tau_l(x_0) = \frac{L^2 - x_0^2}{2D} + \frac{LW}{\pi D} \ln\left[1\Big/\sin\left(\frac{\pi}{2}\frac{w}{W}\right)\right] + \frac{Ll}{D}\frac{W}{w} + \frac{l^2}{2D}, \tag{1.1}$$

where D is the particle diffusivity. Comparison of the mean particle lifetime predicted by the above expression with $\tau_l(x_0)$ obtained from Brownian dynamics simulations shows good agreement between the two when the chamber length L satisfies $L \geqslant 0.5W$.

Researchers face similar two-dimensional diffusion problems in studying various natural and technological processes, for example, transport and reactions on cellular membranes, among others (see Refs. [11–20] and references therein). The difficulties in solving such problems are due to inhomogeneous boundary conditions and varying geometry of the system. Indeed, when the widths of the chamber and the sleeve are equal, $w = W$, the problem of finding the mean particle lifetime becomes essentially one dimensional, and the expression in Eq. (1.1) reduces to the known result [21],

$$\tau_l(x_0)|_{w=W} = \frac{(L+l)^2 - x_0^2}{2D}. \tag{1.2}$$

When deriving Eq. (1.1), we approximately replace the initial problem by an effective one-dimensional one, which can be solved with relative ease. This is explained in the following

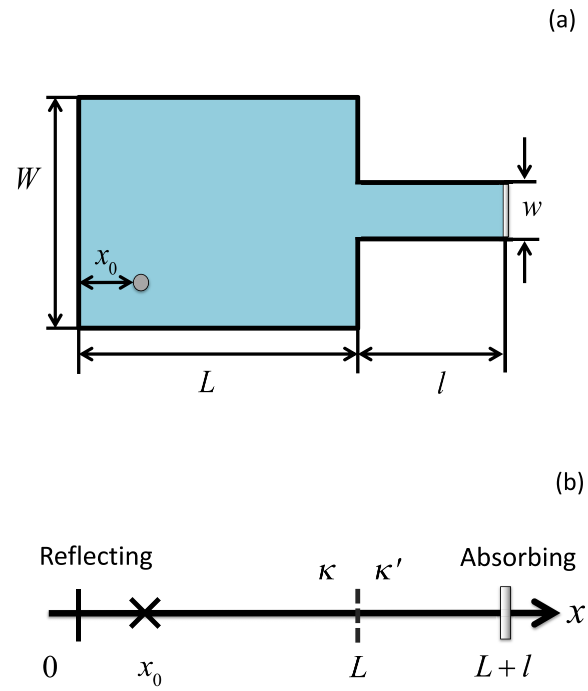

FIG. 1. Rectangular chamber of length L and width W with a sleeve of length l and width $w \leqslant W$ terminated by a binding site (a), and an approximate one-dimensional model of the particle dynamics in the system (b). The particle starting point is located at distance x_0 from the chamber wall opposite to the wall containing the sleeve entrance.

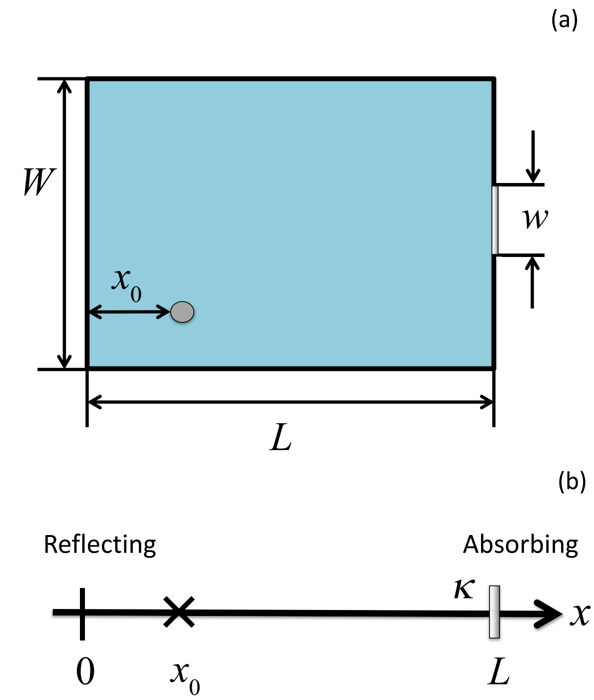

FIG. 2. Rectangular chamber of length L and width W with an absorbing interval of width $w \leqslant W$ located in the center of its right wall (a), and an approximate one-dimensional model of the particle dynamics in the system (b).

Sec. II. Validation of our analytical results by Brownian dynamics simulations is discussed in Sec. III. Some concluding remarks are made in Sec. IV.

II. THEORY

The mean lifetime $\tau_l(x_0)$, Eq. (1.1), is the mean first-passage time of the particle from its starting point in the chamber to the binding site located at the end of the sleeve [see Fig. 1(a)]. To be trapped, the particle first has to enter the sleeve. Therefore, we begin with an approximate one-dimensional description of the particle search for the sleeve entrance. Then we discuss a one-dimensional description of the particle dynamics in the sleeve paying special attention to its return from the sleeve to the chamber. Finally, these two one-dimensional descriptions are used to find $\tau_l(x_0)$.

A. Search for the sleeve entrance

To analyze the particle search for the sleeve entrance one has to solve the two-dimensional diffusion problem in a rectangle of length L and width W with an absorbing interval of length w located in the center of its right wall, as shown in Fig. 2(a). Otherwise, the chamber walls are reflecting. To solve the problem, we use an approximate description that treats the search process as one-dimensional diffusion along the x axis normal to the wall containing the entrance. The diffusion occurs in the interval of length L terminated by reflecting and partially absorbing end points at $x = 0$ and $x = L$, respectively, as illustrated in Fig. 2(b), where x_0 represents the particle starting position. As shown in Sec. III, such a description is justifiable when the chamber length L exceeds its width W. The reason is that in this case in most of the chamber, where x is not too close to L (i.e., to the chamber wall containing the entrance), the two-dimensional distribution function of the particle position depends only on its x coordinate and is constant in the direction normal to the x axis.

Particle trapping by the partially absorbing end point is characterized by the effective trapping rate κ which is a function of the sleeve and chamber widths, w and W. It diverges as $w \to W$ (absorbing boundary at $x = L$) and vanishes as $w \to 0$ (reflecting boundary at $x = L$). This function is given by the Moizhes-Muratov-Shvartsman formula [22,23],

$$\kappa = \frac{\pi D}{W \ln\{1/\sin[\pi w/(2W)]\}}. \tag{2.1}$$

Muratov and Shvartsman [23] proposed this formula in their study of boundary homogenization in the problem of trapping of particles diffusing in a semi-infinite space constrained by a plain boundary periodically, with period W, covered by identical parallel absorbing strips of width $w \leqslant W$. These authors adapted the exact solution of the equivalent electrostatic problem published by Moizhes [22] in 1955.

Naturally, κ in Eq. (2.1) is also an effective trapping rate in the two-dimensional problem of particles diffusing in a semi-infinite plane perpendicular to the striped boundary. In this two-dimensional problem particle motion is restricted by a linear boundary containing alternating absorbing and reflecting intervals of lengths w and $W - w$, respectively.

Because of the symmetry, the latter problem is equivalent to that for particles diffusing in a semi-infinite strip of width W with reflecting side boundaries terminated by a reflecting interval containing an absorbing window of width w in its center. Thus κ in Eq. (2.1) is an exact effective trapping rate for the inhomogeneous boundary constraining such a semi-infinite strip. We use this expression in the case of a finite strip of length L. As shown in Sec. III, the expression works well when $L \geqslant W$.

Having in hand the effective one-dimensional description of diffusion and trapping discussed above, one can find the mean time it takes the particle starting from x_0 to enter the sleeve. This mean time, denoted by $\tau_0(x_0) = \tau_l(x_0)|_{l=0}$, is the sum of the mean first-passage (FP) time from the particle starting point to the chamber wall containing the sleeve entrance, $\tau_{FP}(x_0 \to L)$, and the mean time required for the particle uniformly distributed over this wall (including the entrance) to enter the sleeve, $\tau_0(L)$:

$$\tau_0(x_0) = \tau_{FP}(x_0 \to L) + \tau_0(L). \tag{2.2}$$

These two mean times are given by [21,24]

$$\tau_{FP}(x_0 \to L) = \frac{L^2 - x_0^2}{2D}, \quad \tau_0(L) = \frac{L}{\kappa}. \tag{2.3}$$

Substituting these expressions, with κ given in Eq. (2.1), into Eq. (2.2), we arrive at $\tau_l(x_0)$, Eq. (1.1), with $l = 0$:

$$\tau_0(x_0) = \tau_l(x_0)|_{l=0} = \frac{L^2 - x_0^2}{2D} + \frac{LW}{\pi D} \ln\left[1\Big/\sin\left(\frac{\pi}{2}\frac{w}{W}\right)\right]. \tag{2.4}$$

Which of the two terms, $\tau_{FP}(x_0 \to L)$ or $\tau_0(L)$, dominates depends on both the particle starting distance x_0 and the geometric parameters L, W, and w.

Averaging $\tau_0(x_0)$ over x_0 and assuming that all particle initial positions in the chamber are equally probable, we obtain

$$\langle \tau_0(x_0) \rangle = \frac{1}{L}\int_0^L \tau_0(x_0)dx_0 = \frac{L^2}{3D} + \frac{LW}{\pi D} \ln\left[1\Big/\sin\left(\frac{\pi}{2}\frac{w}{W}\right)\right], \tag{2.5}$$

where the angular brackets $\langle \cdots \rangle$ denote the averaging. A more accurate approximate expression for the averaged mean first-passage time to the absorbing window on the wall of a rectangular chamber is derived in Ref. [15], where it is given in Eq. (99). In contrast to Eq. (2.5) this expression is an infinite sum. One can check that both expressions are identical when the chamber is long enough, and that Eq. (2.5) is simply the first and last terms of the expression in Eq. (99).

In our further analysis we use the above one-dimensional description with the trapping rate κ given by the boundary homogenization, Eq. (2.1), to find the particle mean first-passage time to the binding site at the sleeve end.

B. Dynamics in the sleeve

The particle entering the sleeve either returns to the chamber or gets trapped by the binding site. We assume that its dynamics in the sleeve can be described as one-dimensional diffusion in the interval of length l, $L < x < L + l$, terminated by the absorbing and partially absorbing boundaries at $x = L + l$ and $x = L$, respectively (see Fig. 1). The latter provides an approximate description of the particle escape from the sleeve to the chamber. A similar approach has been used in three dimensions to describe the escape of a particle diffusing in a membrane channel to the bulk reservoir [10,25]. To find the trapping rate κ' entering the boundary condition at $x = L$ [see Fig. 1(b)], consider the case where the sleeve boundary at $x = L + l$ is reflecting and not absorbing. Then the particle distribution in the system approaches equilibrium at long times with the equilibrium two-dimensional density given by $\rho_{eq} = (LW + lw)^{-1}$. The flux entering the sleeve from the chamber at equilibrium is $\rho_{eq} W\kappa$. This flux is compensated by the flux escaping from the sleeve to the chamber, which we assume is given by $\rho_{eq} w\kappa'$. The identity of the two fluxes allows us to establish the relation between the trapping rates κ' and κ,

$$\kappa' w = \kappa W. \tag{2.6}$$

Finally, we find κ' using the expression for κ in Eq. (2.1),

$$\kappa' = \kappa\frac{W}{w} = \frac{\pi D}{w \ln\{1/\sin[\pi w/(2W)]\}}. \tag{2.7}$$

Being furnished with the one-dimensional descriptions of the particle dynamics in the chamber and in the sleeve, we proceed to the derivation of the expression for $\tau_l(x_0)$ in Eq. (1.1).

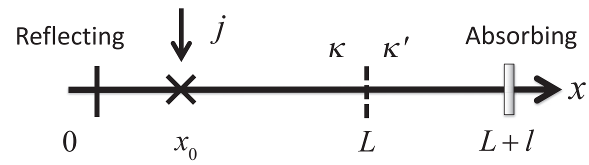

FIG. 3. One-dimensional model used in our derivation of the expression for the mean particle lifetime $\tau_l(x_0)$ given in Eq. (1.1). The derivation exploits the steady-state picture, with the steady state maintained by a constant flux j injected at the particle starting point x_0.

C. Mean lifetime of the particle

To derive Eq. (1.1) consider the steady-state concentration $c(x)$ of diffusing particles in the one-dimensional system of length $L + l$ shown in Fig. 3, where j is a constant flux injected at point x_0, $0 < x_0 < L$. The system consists of two parts representing the chamber, $0 < x < L$, and the sleeve, $L < x < L + l$. The boundary at $x = L$ separating these parts is partially absorbing and characterized by the trapping rates κ and κ' from the chamber and sleeve sides, respectively. The boundary at $x = 0$ is reflecting, whereas the boundary at $x = L + l$ is absorbing. The relation between $\tau_l(x_0)$, the flux j, and the steady-state one-dimensional concentration $c(x)$ is given by

$$\tau_l(x_0) = \frac{1}{j}N, \quad N = \int_0^{L+l} c(x)dx, \tag{2.8}$$

where N is the total number of particles in the system in the steady state. Thus, to find $\tau_l(x_0)$ we need to know the concentration profile $c(x)$.

In the sleeve part of the system $c(x)$ satisfies

$$j = -D\frac{dc(x)}{dx}, \tag{2.9}$$

subject to the absorbing boundary condition at $x = L + l$, $c(L + l) = 0$. Solving Eq. (2.9), we find

$$c(x) = \frac{j}{D}(L + l - x), \quad L < x \leqslant L + l. \tag{2.10}$$

At the boundary separating the two parts of the system, the concentration $c(x)$ makes a jump from $c(L+\varepsilon)|_{\varepsilon\to 0} = jl/D$ to $c(L-\varepsilon)|_{\varepsilon\to 0}$. The jump magnitude is determined from the flux conservation requirement,

$$j = \kappa c(L-\varepsilon)|_{\varepsilon\to 0} - \kappa' c(L+\varepsilon)|_{\varepsilon\to 0}. \tag{2.11}$$

We use this together with Eq. (2.7) to find $c(L-\varepsilon)|_{\varepsilon\to 0}$:

$$c(L-\varepsilon)|_{\varepsilon\to 0} = \frac{1}{\kappa}(j + \kappa' c(L+\varepsilon)|_{\varepsilon\to 0}) = \frac{j}{D}\left(\frac{W}{w}l + \frac{D}{\kappa}\right). \tag{2.12}$$

In the chamber part of the system, the concentration satisfies Eq. (2.9) with $c(L-\varepsilon)|_{\varepsilon\to 0}$ given in Eq. (2.12), when $x_0 < x < L$, and remains constant, equal to $c(x_0)$, when $0 \leqslant x < x_0$. Solving Eq. (2.9), we obtain

$$c(x) = \frac{j}{D}\left(\frac{W}{w}l + \frac{D}{\kappa} + L - x_0 H(x_0 - x) - xH(x - x_0)\right),$$
$$0 < x \leqslant L, \tag{2.13}$$

where $H(z)$ is the Heaviside step function.

To find $\tau_l(x_0)$ it remains to calculate the total number of particles N by performing the integration of $c(x)$ over x, Eq. (2.8), and then find the ratio N/j. One can check that this leads to the expression for $\tau_l(x_0)$ in Eq. (1.1), which is one of the main results of this work. Averaging $\tau_l(x_0)$ over x_0, assuming that all particle initial positions in the chamber are equally probable, we arrive at

$$\langle \tau_l(x_0)\rangle = \frac{L^2}{3D} + \frac{LW}{\pi D}\ln\left[1\Big/\sin\left(\frac{\pi}{2}\frac{w}{W}\right)\right] + \frac{Ll}{D}\frac{W}{w} + \frac{l^2}{2D}. \tag{2.14}$$

This is another main result of the present study.

III. BROWNIAN DYNAMICS SIMULATIONS

In this section we compare our approximate analytical results for the mean times $\tau_0(x_0)$ and $\tau_l(x_0)$ with corresponding results obtained from two-dimensional Brownian dynamics simulations for $x_0 = L$. The goal is to test the accuracy of our theoretical predictions and to establish the range of their applicability as functions of the geometric parameters L, W, l, and w characterizing the system. We begin with the mean search time $\tau_0(x_0)$ and then proceed to the mean lifetime $\tau_l(x_0)$.

A. Search for the sleeve entrance

The expressions in Eqs. (2.2) and (2.4) present the mean search time $\tau_0(x_0)$ as the sum of two terms: $\tau_{FP}(x_0 \to L)$ and $\tau_0(L)$, which are given in Eq. (2.3). It is assumed that the starting point of the particle is uniformly distributed over the channel width as fixed x_0. Then the presentation of $\tau_0(x_0)$ as the sum and the expression for $\tau_{FP}(x_0 \to L)$, Eq. (2.3), are exact results, while the expression for $\tau_0(L)$ is an approximation derived by imposing the radiation boundary condition at $x = L$ with the trapping rate κ, Eq. (2.1), obtained using boundary homogenization. To test the accuracy of this expression and to establish the range of its applicability, we compare $\tau_0(L)$ predicted by the theory and obtained from Brownian dynamics simulations. According to Eq. (2.4) we have

TABLE I. The relative error in per cents of our approximate analytical expression for the mean particle lifetime $\tau_0(L)$, Eq. (3.1), in a rectangular chamber of length L and width W with an absorbing window of width from Brownian dynamics simulations for three values of the window size, $w/W = 0.25$, 0.5, and 0.75, and six values of the chamber length, $L/W = 0.25$, 0.5, 0.75, 1.0, 2.0, and 3.0.

		L/W					
		0.25	0.50	0.75	1.0	2.0	3.0
	0.25	8.78	1.75	1.94	1.59	1.55	2.27
w/W	0.50	8.27	2.24	1.51	1.22	0.97	0.56
	0.75	5.71	2.27	2.20	2.13	1.98	1.83

$$\tau_0(L) = \frac{L}{\kappa} = \frac{LW}{\pi D}\ln\left[1\Big/\sin\left(\frac{\pi}{2}\frac{w}{W}\right)\right]. \tag{3.1}$$

This time was compared with its counterpart obtained from Brownian dynamics simulations. The relative error of our theoretical predictions is presented in Table I for three values of the sleeve entrance width, $w/W = 0.25$, 0.5, and 0.75, and six values of the chamber length, $L/W = 0.25$, 0.5, 0.75, 1.0, 2.0, and 3.0.

In our simulations we run $N = 200000$ trajectories whose starting points are uniformly distributed over the chamber wall containing the sleeve entrance. A trajectory is terminated as soon as it crosses the entrance for the first time. The mean search time, denoted by $\tau_0^{(\mathrm{sim})}(L)$, is defined as

$$\tau_0^{(\mathrm{sim})}(L) = \frac{1}{N}\sum_{i=1}^{N} t_i, \tag{3.2}$$

where t_i is the lifetime of the ith trajectory. For trajectories starting from the entrance this lifetime is zero. Thus, the number of trajectories with non-zero lifetime is $N(1 - w/W)$. The results presented in Table I show that Eq. (3.1) predicts $\tau_0(L)$ with high accuracy (the relative error less than 3%) when the chamber length exceeds half of its width, $L \geqslant 0.5W$, and fails for shorter chambers, $L < 0.5W$. This should be expected since the derivation of Eq. (3.1) is based on the Moizhes-Muratov-Shvartsman formula for κ, Eq. (2.1), obtained for the semi-infinite system as mentioned above.

B. Mean lifetime of the particle

The expression in Eq. (1.1) presents the mean lifetime $\tau_l(x_0)$ as the sum of four terms, which have transparent physical interpretations. The first two terms give the mean time it takes the particle to enter the sleeve from the chamber, $\tau_0(x_0)$, whereas the last two terms give the mean lifetime of a particle

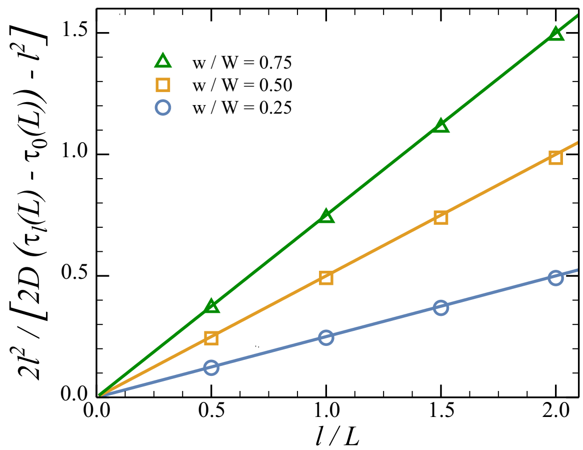

FIG. 4. Numerical test of the l dependence of the mean particle lifetime $\tau_l(x_0)$, Eq. (1.1). To test the l dependence predicted by Eq. (1.1) we wrote this equation in the form given in Eq. (3.4). The straight lines in the figure are the linear dependence on l/L in the right-hand side of Eq. (3.4) for three values of the slope, $w/W = 0.25$, 0.5, and 0.75 from bottom to top. Symbols are the values of the expression on the left-hand side of Eq. (3.4) found for $x_0 = L$ using the mean lifetimes $\tau_l^{(\mathrm{sim})}(L)$ obtained from Brownian dynamics simulations and $\tau_0(L)$ given in Eq. (3.1).

entering the sleeve, i.e., starting from the sleeve entrance. Thus, we have

$$\tau_l(x_0) = \tau_0(x_0) + \frac{Ll}{D}\frac{W}{w} + \frac{l^2}{2D}, \tag{3.3}$$

The last term in this equation, $l^2/(2D)$, is the mean particle lifetime on condition that the sleeve entrance is a reflecting boundary, i.e., a particle entering the sleeve never returns to the chamber. The second term, $LlW/(Dw)$, can be interpreted as the mean time spent by the particle on those segments of the trajectories that escape from the sleeve to the chamber and then come back to the sleeve.

As shown above, our formalism based on the boundary homogenization provides an accurate description of $\tau_0(x_0)$, Eq. (2.4), when the chamber length satisfies $L \geqslant 0.5W$. Now the focus is on the l dependence of the mean lifetime $\tau_l(x_0)$ on condition that the chamber is long enough. To this end, we rewrite Eq. (3.3) as

$$\frac{2l^2}{2D(\tau_l(x_0) - \tau_0(x_0)) - l^2} = \frac{w}{W}\frac{l}{L}, \tag{3.4}$$

and test this relation at $L = W$ using $\tau_0(x_0)$ given in Eq. (2.4) and $\tau_l(x_0)$ obtained from Brownian dynamics simulations.

In simulations we run $N = 200000$ trajectories whose starting points are uniformly distributed over the chamber wall containing the sleeve entrance, $x_0 = L$. The trajectories are terminated as soon as they touch the absorbing end of the sleeve located at $x = L + l$ [see Fig. 1(a)] for the first time. The mean particle lifetime, denoted by $\tau_l^{(\mathrm{sim})}(x_0)$, is defined as

$$\tau_l^{(\mathrm{sim})}(x_0) = \frac{1}{N}\sum_{i=1}^{N} t_i, \tag{3.5}$$

where t_i is the lifetime of the ith trajectory. The simulations were run for three values of the sleeve entrance width, $w/W = 0.25$, 0.5, and 0.75, and four values of the sleeve length, $l/L = 0.5$, 1.0, 1.5, and 2.0. According to Eq. (3.3) the difference $\tau_l(x_0) - \tau_0(x_0)$ is independent of x_0. Keeping this in mind, for our simulations we chose $x_0 = L$.

The comparison of the theoretical predictions with the simulation results is presented in Fig. 4, where the three straight lines are the linear dependences on the ratio l/L on the right-hand side of Eq. (3.4) with the slopes $w/W = 0.25$, 0.5, and 0.75. The symbols are the values of the left-hand side of this equation found using the mean lifetimes $\tau_l^{(\mathrm{sim})}(L)$ obtained from Brownian dynamics simulations and $\tau_0(L)$ given in Eq. (3.1). One can see excellent agreement between the theoretical predictions and the simulation results.

IV. DISCUSSION AND CONCLUDING REMARKS

Our analysis of trapping of diffusing particles by a hidden binding site is based on the reduction of the initial two-dimensional problem to the effective one-dimensional one (see Fig. 1). A specific feature of the geometry shown in Fig. 1(a) is the abrupt change of the channel width. This makes it impossible to use conventional reduction to a one-dimensional description in terms of the generalized Fick-Jacobs equation [26–34]. To bypass this difficulty, we took advantage of the approximation based on boundary homogenization, which treats crossing the point where the channel width changes abruptly as trapping by a partially absorbing boundary. This approach has been used earlier in three dimensions [35–37]. Here, we apply it for the analysis of a two-dimensional problem. Kalinay and Percus [38] validated this approximation in both two and three dimensions by analytical consideration.

One of the main results of the present work is the expression in Eq. (1.1) which shows how the mean particle lifetime $\tau_l(x_0)$ depends on the geometric parameters of the system, L, W, l, and w, as well as the particle initial position x_0. Abrupt change in the system width results in a slowdown of the trapping kinetics and hence the increase of the mean particle lifetime. The difference between $\tau_l(x_0)$ and its counterpart in the absence of the abrupt width change $\tau_l(x_0)|_{w=W}$, Eq. (1.2), is given by

$$\tau_l(x_0) - \tau_l(x_0)|_{w=W} = \frac{LW}{D}\left\{\frac{1}{\pi}\ln\left[1\Big/\sin\left(\frac{\pi}{2}\frac{w}{W}\right)\right] + \frac{l}{w}\left(1 - \frac{w}{W}\right)\right\}. \tag{4.1}$$

The two terms in the curly brackets have different origins. The first term, which is independent of the sleeve length l, is associated with the first particle entry into the sleeve. The second term, proportional to l, is associated with segments of the particle trajectory returning to the chamber from the sleeve. Because of the abrupt width change these fragments stay in the chamber longer than their counterparts in the absence of the width change. Which of the two terms dominates is controlled by the two dimensionless parameters, w/W and l/w. The first term dominates in the case of short sleeves, where the sleeve length satisfies

$$l \ll \frac{w}{\pi}\ln\left[1\Big/\sin\left(\frac{\pi}{2}\frac{w}{W}\right)\right]\Big/\sin\left(\frac{\pi}{2}\frac{w}{W}\right)\Big/\left(1-\frac{w}{W}\right). \tag{4.2}$$

In the opposite limiting case, the delay time due to the width jump is determined by the second term.

Another result of this work is a general methodology developed on the basis of the method of boundary homogenization. We hope that this methodology will be used in the future to analyze diffusive transport in two-dimensional systems with abruptly changing width.

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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