Trapping of diffusing particles by striped cylindrical surfaces. Boundary homogenization approach

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We study trapping of diffusing particles by a cylindrical surface formed by rolling a flat surface, containing alternating absorbing and reflecting stripes, into a tube. For an arbitrary stripe orientation with respect to the tube axis, this problem is intractable analytically because it requires dealing with non-uniform boundary conditions. To bypass this difficulty, we use a boundary homogenization approach which replaces non-uniform boundary conditions on the tube wall by an effective uniform partially absorbing boundary condition with properly chosen effective trapping rate. We demonstrate that the exact solution for the effective trapping rate, known for a flat, striped surface, works very well when this surface is rolled into a cylindrical tube. This is shown for both internal and external problems, where the particles diffuse inside and outside the striped tube, at three orientations of the stripe direction with respect to the tube axis: (a) perpendicular to the axis, (b) parallel to the axis, and (c) at the angle of $\pi/4$ to the axis. © 2015 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4922444>]

I. INTRODUCTION

The problem of trapping of diffusing particles by heterogeneous boundaries, with absorbing regions on the otherwise reflecting surfaces, arises in the analysis of various processes in physics, chemistry, and biology. Examples include electric current through arrays of microelectrodes,^{1–3} porous membrane transport,^{4–6} reactions on supported catalysts,⁷ water exchange in plants,⁸ ligand binding to cell surface receptors,^{9–18} ligand accumulation in cell culture assays,^{19,20} to mention just a few. This is an extremely complicated problem, because it involves non-uniform boundary conditions on the surface. This difficulty can be overcome by using an approximate effective-medium-type approach called boundary homogenization.

The approach exploits the fact that the fields of the particle fluxes and concentrations become uniform in the lateral direction as the distance from the boundary surface increases. As a consequence, sufficiently far from the surface, these fields are indistinguishable from those when the surface is uniformly partially absorbing with a properly chosen effective trapping rate. With this in mind, one can replace the non-uniform boundary conditions on the surface by an effective homogeneous one. This procedure of introducing the effective boundary condition, called boundary homogenization, significantly simplifies the initial problem.

To implement this approach, one needs to know the effective trapping rate that characterizes the trapping efficiency of the homogenized boundary, which depends on the shape and size of the absorbing regions as well as on their distribution on the surface. The effective trapping rate, as a function of the surface properties, is known only in a few special cases. For example, the Berg-Purcell-Shoup-Szabo formula^{9,10} gives the effective trapping rate for a surface randomly covered by identical, small, absorbing circular disks in the limiting case of

low disk surface fraction. The effective trapping rates in more complex situations can be obtained by means of computer-assisted boundary homogenization, as discussed in recent papers.^{21–25}

Periodically striped, flat surfaces, formed by identical, equally spaced absorbing stripes on the otherwise reflecting surface (see Fig. 1), are a unique example, where there is a simple analytical expression for the effective trapping rate, which is valid for all values of the stripe surface fraction. Let L and l be the period and the width of individual absorbing stripes, respectively (see Fig. 1), so that the stripe surface fraction, σ , is

$$\sigma = \frac{l}{L}. \quad (1.1)$$

The effective trapping rate, κ_{eff} , as a function of σ and l or L is given by²⁵

$$\kappa_{eff} = \frac{\pi D \sigma}{l \ln [1 / \sin (\pi \sigma / 2)]} = \frac{\pi D}{L \ln [1 / \sin (\pi \sigma / 2)]}, \quad (1.2)$$

where D is the particle diffusion constant. This formula shows (i) that the effective trapping rate approaches zero, as $\sigma \rightarrow 0$ at a fixed value of the period L , as $1 / \ln (1 / \sigma)$, and (ii) that the surface becomes perfectly absorbing ($\kappa_{eff} \rightarrow \infty$) both as $\sigma \rightarrow 1$ and as $l \rightarrow 0$ for any value of σ . The result for the effective trapping rate in Eq. (1.2) was first published by Muratov and Shvartsman,²⁵ who used the exact solution of the equivalent electrostatic problem obtained by Moizhes²⁶ about six decades ago.

The expression in Eq. (1.2) gives the effective trapping rate by a periodically striped, flat surface. In this paper, we use Brownian dynamics simulations to study the applicability of κ_{eff} in Eq. (1.2) to the problem of trapping of diffusing particles by periodically striped cylindrical surfaces which

FIG. 1. Schematic representation of flat, periodically striped surfaces of period L , formed by identical, equally spaced absorbing stripes of length l on the otherwise reflecting surface.

are formed by rolling periodically striped, flat sheets into cylindrical tubes. Three orientations of the stripe direction with respect to the tube axis are considered (see Fig. 2): (a) perpendicular to the axis, (b) parallel to the axis, and (c) at the angle of $\pi/4$ to the axis. For each orientation, we study both internal and external problems, where the particles diffuse inside and outside the striped tube, respectively. From Brownian dynamics simulations, we obtain the mean particle lifetimes. These times are compared with theoretically predicted mean particle lifetimes for the tubes with homogenized boundary conditions on the tube walls, assuming that the effective wall trapping rates are identical to those for the corresponding flat surfaces and given by Eq. (1.2). This comparison shows that Eq. (1.2) provides an accurate description of the effective homogeneous trapping rate by periodically striped cylindrical surfaces over the entire range of the stripe surface fraction in both internal and external problems for all three stripe orientations.

The outline of the paper is as follows. In Sec. III, we compare the mean lifetimes obtained from Brownian dynamics simulations with their theoretically predicted counterparts which are discussed in Sec. II. Section IV contains a summary of the obtained results and some concluding remarks. In this section, we propose a hypothesis that the effective trapping rate κ_{eff} in Eq. (1.2) is an intrinsic property of the periodically striped surface. Therefore, it can be used for an arbitrary orientation of the stripes with respect to the tube axis.

FIG. 2. Schematic representation of periodically striped cylindrical surfaces with three different orientations of the stripe direction with respect to the tube axis, perpendicular to the axis (panel (a)), parallel to the axis (panel (b)), and at the angle of $\pi/4$ to the axis (panel (c)).

II. PRELIMINARIES

In this section, we explain how the theoretical expressions for the mean lifetimes, which are used for comparison with the simulation results, can be obtained for the internal (*in*) and external (*ex*) problems. Our discussion below exploits the fact that after boundary homogenization, the trapping problem in a striped cylindrical tube becomes effectively one-dimensional.

A. Internal problem

Consider a point particle diffusing in a circular disk of radius R with a uniform partially absorbing boundary characterized by a trapping rate κ . Let $\tau_{in}(r)$ be the mean lifetime of such a particle that starts at distance r from the disk center located at the origin, $r \leq R$. This time, considered as a function of r , satisfies^{27,28}

$$\frac{d}{dr} \left(r \frac{d\tau_{in}(r)}{dr} \right) = -\frac{r}{D}, \quad (2.1)$$

subject to the reflecting boundary condition at the origin and radiation boundary condition at $r = R$,

$$\left. \frac{d\tau_{in}(r)}{dr} \right|_{r=0} = 0, \quad -D \left. \frac{d\tau_{in}(r)}{dr} \right|_{r=R} = \kappa \tau_{in}(R). \quad (2.2)$$

Integrating Eq. (2.1), one arrives at an intuitively appealing formula according to which the mean lifetime $\tau_{in}(r)$ is the sum of the mean first-passage (FP) time to the disk boundary from the particle starting point, $\tau_{FP}(r \rightarrow R)$, and the mean lifetime of the particle when it starts from the boundary, $\tau_{in}(R)$,

$$\tau_{in}(r) = \tau_{FP}(r \rightarrow R) + \tau_{in}(R). \quad (2.3)$$

These two mean times are given by

$$\tau_{FP}(r \rightarrow R) = \frac{1}{4D} (R^2 - r^2) \quad (2.4)$$

and

$$\tau_{in}(R) = \frac{R}{2\kappa}. \quad (2.5)$$

Assuming a uniform distribution of the particle starting point over the disk area, and averaging the mean lifetime $\tau_{in}(r)$ over r , one finds the averaged mean lifetime, denoted by τ_{in} ,

$$\tau_{in} = \frac{2}{R^2} \int_0^R \tau_{in}(r) r dr = \frac{R^2}{8D} + \frac{R}{2\kappa}. \quad (2.6)$$

In our three-dimensional Brownian dynamics simulations of the internal problem, we obtain the mean lifetime of the particle, whose starting point is uniformly distributed inside a periodically striped tube. This lifetime denoted by τ_{in}^{sim} is compared with τ_{in} in Eq. (2.6) with $\kappa = \kappa_{eff}$, where κ_{eff} is the effective trapping rate in Eq. (1.2) for the corresponding flat, striped surface.

B. External problem

Consider a point particle diffusing in the annulus bounded by two concentric circles of radii R and R_{out} , $R_{out} > R$. It is assumed that the outer circle of radius R_{out} is a reflecting boundary for the particle, while the inner circle of radius R

is a uniform partially absorbing boundary characterized by a trapping rate κ . Let $\tau_{ex}(r)$ be the mean lifetime of a particle that starts at distance r from the circle center located at the origin, $R \leq r \leq R_{out}$. Time $\tau_{ex}(r)$ satisfies Eq. (2.1), subject to the reflecting boundary condition at $r = R_{out}$ and radiation boundary condition at $r = R$,

$$\left. \frac{d\tau_{ex}(r)}{dr} \right|_{r=R_{out}} = 0, \quad D \left. \frac{d\tau_{ex}(r)}{dr} \right|_{r=R} = \kappa \tau_{ex}(R). \quad (2.7)$$

Integrating the equation, one obtains

$$\tau_{ex}(r) = \tau_{FP}(r \rightarrow R) + \tau_{ex}(R), \quad (2.8)$$

where $\tau_{FP}(r \rightarrow R)$ is the particle mean first-passage time to the inner circle, and $\tau_{ex}(R)$ is the mean lifetime of the particle starting from the inner circle. These mean times are given by

$$\tau_{FP}(r \rightarrow R) = \frac{1}{4D} \left[2R_{out}^2 \ln \left(\frac{r}{R} \right) - r^2 + R^2 \right] \quad (2.9)$$

and

$$\tau_{ex}(R) = \frac{R_{out}^2 - R^2}{2\kappa R}. \quad (2.10)$$

In our three-dimensional Brownian dynamics simulations of the external problem, we study particles diffusing between two concentric cylindrical tubes of radii R and R_{out} , $R_{out} > R$. The particles can be trapped by the inner, periodically striped tube, while the outer tube is a reflecting boundary. From the simulations, we obtain the mean lifetime, τ_{ex}^{sim} , of a particle whose starting point is uniformly distributed over the inner tube surface. This lifetime is compared with $\tau_{ex}(R)$ in Eq. (2.10) with $\kappa = \kappa_{eff}$, where κ_{eff} is the effective trapping rate in Eq. (1.2) for the corresponding flat, striped surface.

III. RESULTS AND DISCUSSIONS

In this section, we compare the mean particle lifetimes obtained from Brownian dynamics simulations and those predicted by the theory which is based on boundary homogenization. This is done for both internal and external problems with the three stripe orientations with respect to the tube axis, shown in Fig. 2. The goal is to study the applicability of the expression for the effective trapping rate in Eq. (1.2), which is an exact result for the flat geometry, in the case of cylindrical geometry. Our estimates show that the relative error of the mean particle lifetimes obtained from the simulations does not exceed 3%.

A. Stripes perpendicular to the tube axis

When the stripes are perpendicular to the tube axis (see Fig. 2(a)), the system is characterized by two dimensionless parameters: the stripe surface fraction, $\sigma = l/L$, and the ratio of the stripe period to the tube radius, L/R . In our Brownian dynamics simulations of the internal problem, we determine the mean particle lifetime, τ_{in}^{sim} , which is compared with its counterpart in Eq. (2.6), where $\kappa = \kappa_{eff}$ given by Eq. (1.2). The results are presented in Table I that gives the ratios $\tau_{in}^{sim}/\tau_{in}$ for different values of the parameters σ and L/R . One can see that the relative error of the theoretical predictions does not exceed 3%.

TABLE I. The ratios of the mean lifetimes τ_{in}^{sim} obtained from the simulations of the internal problem in the geometry shown in Fig. 2(a) to their counterparts τ_{in} in Eq. (2.6), where $\kappa = \kappa_{eff}$ for the corresponding flat surfaces given by Eq. (1.2).

L/R	$\sigma = l/L$					
	0.05	0.1	0.2	0.4	0.6	0.8
0.125	0.992	0.993	1.007	0.997	0.996	0.999
0.25	0.995	1.020	1.005	0.991	0.990	0.998
0.5	1.017	1.023	1.024	1.018	1.012	1.001
1	1.020	1.024	1.022	1.015	1.016	0.993
1.5	1.019	1.017	1.022	1.020	1.018	0.992
2	1.022	1.021	0.986	1.012	1.011	1.005
5	1.022	1.021	0.986	1.012	1.011	1.005
10	1.021	1.017	1.027	1.020	0.977	1.013

When studying the external problem (see Fig. 3), we analyze the ratios of the mean lifetimes obtained from the simulations and predicted by the theory, $\tau_{ex}^{sim}/\tau_{ex}$, for four values of the stripe surface fractions, $\sigma = 0.2, 0.4, 0.6$, and 0.8 , taking the stripe period equal to the tube radius, $L = R$. This is done for several values of the outer tube radius, R_{out} . The results are summarized in Table II. One can see that the relative error of the theoretical predictions depends on the value of R_{out} . The relative error does not exceed 3% for $R_{out} \geq 1.4R$, while it can be much larger for smaller values of R_{out} . This is not surprising because boundary homogenization is applicable only if the distances between the inner and outer tubes are sufficiently large. The requirement $R_{out} \geq 1.4R$ establishes the condition of applicability of the boundary homogenization approach in the external problem shown in Fig. 3.

B. Stripes parallel to the tube axis

When the stripes are parallel to the tube axis (see Fig. 2(b)), the tube radius R cannot be arbitrary. A tube rolled from a periodically striped flat surface of period L is also periodic only when its radius R satisfies

$$R = \frac{nL}{2\pi}, \quad (3.1)$$

where n is the number of stripes on the tube surface, $n = 1, 2, 3, \dots$. In addition, when the stripes are parallel to the tube axis, the system is invariant with respect to translations in the tube axis direction. Therefore, in this case we run two-dimensional Brownian dynamics simulations in the plane orthogonal to the tube axis.

FIG. 3. Schematic representation of two concentric cylindrical tubes of radii R and R_{out} , $R_{out} > R$. The internal tube contains periodic shaded rings orthogonal to the tube axis, which absorb diffusing particles.

TABLE II. The ratios of the mean lifetimes τ_{ex}^{sim} obtained from the simulations in the geometry shown in Fig. 3 to their counterparts $\tau_{ex}(R)$ in Eq. (2.10), where $\kappa = \kappa_{eff}$ for the corresponding flat surfaces given by Eq. (1.2).

R_{out}/R	$\sigma = l/L$			
	0.2	0.4	0.6	0.8
1.1	1.132	1.201	1.110	0.967
1.2	1.130	1.128	1.078	1.000
1.4	0.976	0.975	0.983	0.978
1.6	0.982	0.982	0.991	0.986
1.8	0.981	0.984	0.988	0.992
2	0.981	0.985	0.980	0.995

TABLE III. The ratios of the mean lifetimes τ_{in}^{sim} obtained from the simulations of the internal problem for a disk of radius R with $n = 2\pi R/L$ evenly spaced absorbing arcs of length l , which occupy fraction $\sigma = nl/(2\pi R) = l/L$ of the disk perimeter, to their counterparts τ_{in} in Eq. (2.6), where $\kappa = \kappa_{eff}$ for the corresponding flat surfaces given by Eq. (1.2).

n	$\sigma = l/L = nl/(2\pi R)$					
	0.05	0.1	0.2	0.4	0.6	0.8
1	1.007	1.000	0.996	1.018	1.010	1.009
2	1.012	1.007	1.012	1.016	1.004	0.993
3	1.009	1.013	1.011	0.987	1.002	1.010
4	1.017	0.999	1.001	1.001	1.016	1.013

When studying the internal problem, the simulations were run inside a circular disk of radius R , containing $n = 1, 2, 3$, and 4 identical, evenly spaced absorbing arcs of length l (see Fig. 4(a)). The arc line fraction, $nl/(2\pi R)$, is identical to the stripe surface fraction and given by

$$\sigma = \frac{l}{L} = \frac{nl}{2\pi R}. \quad (3.2)$$

The mean particle lifetime, τ_{in}^{sim} , obtained from the simulations is compared with its counterpart in Eq. (2.6), where $\kappa = \kappa_{eff}$ given by Eq. (1.2). The values of the lifetime ratio $\tau_{in}^{sim}/\tau_{in}$ obtained for different n and σ are summarized in Table III. One can see that the relative error of the theoretical predictions does not exceed 3%. Voituriez²⁹ drew our attention to the fact that in the case of only one absorbing stripe, Eq. (2.6) with $\kappa = \kappa_{eff}$ provides an exact solution for τ_{in} , obtained by Singer *et al.*³⁰

FIG. 4. A disk of radius R (panel (a)) and an annuli bounded by the inner and outer circles of radii R and R_{out} , $R_{out} > R$, used in the simulations of the internal and external problems with $n = 3$, respectively. The three identical, evenly spaced absorbing arcs of length l occupy the line fraction $\sigma = 3l/(2\pi R) = l/L$ of the disk boundary in panel (a) and of the inner circle in panel (b).

When studying the external problem, Brownian dynamics simulations were run in annuli bounded by the inner circle of radius R and outer circles of different radii R_{out} . The inner circle contains n identical, evenly spaced absorbing arcs, $n = 1, 2, 3$, and 4, of length l , whereas the outer circles are always reflecting boundaries for diffusing particles (see Fig. 4(b)). The mean particle lifetimes, τ_{ex}^{sim} , obtained from the simulations are compared with their theoretically predicted counterparts, $\tau_{ex}(R)$, given by Eq. (2.10), where $\kappa = \kappa_{eff}$ in Eq. (1.2). The ratios of these mean lifetimes for several values of the outer circle radius R_{out} are presented in Table IV for $\sigma = 0.2, 0.4, 0.6$, and 0.8. One can see that the relative error of the theoretical predictions does not exceed 3% for $R_{out} \geq 3R$. This inequality establishes the condition of applicability of the boundary homogenization in the external problem for the two-dimensional geometry shown in Fig. 4(b). For $R_{out} < 3R$, the relative error rapidly increases as the outer circle radius decreases, because boundary homogenization is not applicable in this range of the outer circle radius.

A very detailed analysis of trapping by a circle with identical, evenly spaced absorbing arcs of arbitrary length can be found in a recent paper by Rupprecht *et al.*³¹ Their study provides the exact analytical solutions for both internal and external problems, which are rather complicated. The result for the mean particle lifetime in the internal problem, given in Eq. (29) from Ref. 31, is identical to our expression in Eq. (2.6) with $\kappa = \kappa_{eff}$. Thus, the boundary homogenization approach provides an exact solution for τ_{in} not only for one absorbing stripe, as mentioned earlier, but also for an arbitrary

TABLE IV. The ratios of the mean lifetimes τ_{ex}^{sim} obtained from the simulations of the external problem in the annuli between the reflecting outer circle of radius R_{out} and the inner circle of radius R , containing n identical evenly spaced absorbing arcs of length l , to their counterparts $\tau_{ex}(R)$ in Eq. (2.10), where $\kappa = \kappa_{eff}$ for the corresponding flat surfaces given by Eq. (1.2).

R_{out}/R	$\sigma = l/L = nl/(2\pi R)$			
	0.2	0.4	0.6	0.8
$n = 1$				
1.5	1.599	1.505	1.302	1.325
2.0	0.915	1.065	1.118	1.124
2.5	0.975	1.020	1.037	1.063
3.0	0.986	0.989	0.986	1.015
$n = 2$				
1.5	2.313	2.166	1.626	1.022
2.0	0.970	0.911	1.033	0.973
2.5	1.029	1.029	1.026	1.025
3.0	1.028	1.024	1.017	1.022
$n = 3$				
1.5	3.488	3.250	2.412	1.283
2.0	1.467	1.374	1.007	1.026
2.5	1.029	0.975	1.028	1.022
3.0	1.015	1.018	1.025	1.018
$n = 4$				
1.5	4.643	4.314	3.214	1.706
2.0	1.938	1.807	1.346	1.028
2.5	1.109	1.037	0.777	0.978
3.0	0.984	1.016	1.024	1.017

TABLE V. The ratios of the mean lifetimes τ_{in}^{sim} obtained from the simulations of the internal problem in the geometry shown in Fig. 2(c) to their counterparts τ_{in} in Eq. (2.6), where $\kappa = \kappa_{eff}$ for the corresponding flat surfaces given by Eq. (1.2).

$\sigma = l/L$					
0.05	0.1	0.2	0.4	0.6	0.8
0.972	0.973	0.970	0.977	0.985	0.988

number of stripes. It is worth noting that although the analysis in the framework of the boundary homogenization approach has an advantage of being simple, it also has a disadvantage of being limited by the requirement that the outer circle must be sufficiently far from the inner one. At the same time, the exact solution obtained in Ref. 31 is free from this restriction.

Boundary homogenization has been applied to study the mean lifetime of particles diffusing inside a circle with identical, evenly spaced absorbing arcs on its boundary (internal problem) in Ref. 32. In this work, the authors used an approximate expression for the effective trapping rate, proposed in Ref. 23, which we denote by κ_{eff}^{approx} ,

$$\kappa_{eff}^{approx} = \frac{nD}{2R(1-\sigma)^2 \ln(2.6 + 0.7/\sigma)} = \frac{\pi D \sigma}{l(1-\sigma)^2 \ln(2.6 + 0.7/\sigma)}. \quad (3.3)$$

They found good agreement between the mean lifetimes given by Eq. (2.6) with $\kappa = \kappa_{eff}^{approx}$ and those obtained by numerically solving the two-dimensional diffusion equation with non-uniform boundary conditions. Note that, although the two expressions for the effective trapping rate, Eqs. (1.2) and (3.3), look significantly different, the ratio, $\kappa_{eff}^{approx}/\kappa_{eff}$, considered as a function of σ does not exceed 1.05.

C. Stripes at the angle $\pi/4$ with respect to the tube axis

When the stripe direction forms angle θ with the tube axis, this angle, the period L of the striped surface forming the tube wall, and the tube period, L_{tube} , in the tube axis direction are related by the following relationship:

$$L_{tube} = \frac{L}{\sin \theta}. \quad (3.4)$$

TABLE VI. The ratios of the mean lifetimes τ_{ex}^{sim} , obtained from the simulations in the geometry shown in Fig. 5 to their counterparts $\tau_{ex}(R)$ in Eq. (2.10), where $\kappa = \kappa_{eff}$ for the corresponding flat surfaces given by Eq. (1.2).

R_{out}/R	$\sigma = l/L$			
	0.2	0.4	0.6	0.8
1.1	1.297	1.032	1.110	0.967
1.2	1.024	1.128	1.078	1.000
1.4	0.976	0.975	0.983	0.978
1.6	0.982	0.982	0.991	0.986
1.8	0.981	0.984	0.988	0.992
2	0.981	0.985	0.980	0.995

FIG. 5. Schematic representation of two concentric cylindrical tubes of radii R and R_{out} , $R_{out} > R$. The internal tube contains a shaded stripe making the angle $\pi/4$ with the tube axis, which absorbs diffusing particles.

This shows that the two periods are equal, $L_{tube} = L$, when $\theta = \pi/2$, i.e., for stripes perpendicular to the tube axis, whereas for stripes parallel to the tube axis, $L_{tube} = \infty$. The tube radius R , the surface period L , and the angle θ are related by

$$2\pi R \cos \theta = Ln, \quad (3.5)$$

which is a generalization of the relation in Eq. (3.1) for stripes parallel to the tube axis to the case of arbitrary angle θ formed by the periodic stripes with the tube axis. The relation in Eq. (3.5) does not work for strips perpendicular to the tube axis ($\theta = \pi/2$), where the tube radius can be arbitrary.

In our Brownian dynamics simulations, we study the simplest case of $n = 1$ and $\theta = \pi/4$ (see Fig. 2(c)), where Eqs. (3.4) and (3.5) reduce to

$$L_{tube} = \sqrt{2}L, \quad R = \frac{L}{\pi\sqrt{2}}. \quad (3.6)$$

The ratios of the mean particle lifetimes obtained from the simulations and predicted by the theory for the internal and the external problems, $\tau_{in}^{sim}/\tau_{in}$ and $\tau_{ex}^{sim}/\tau_{ex}(R)$, are presented in Tables V and VI, respectively. The simulations of the external problem were performed for several values of R_{out} (see Fig. 5) to establish the range of applicability of boundary homogenization in this geometry. One can see that the relative error of the theoretical predictions does not exceed 3% in both cases when the outside radius satisfies $R_{out} \geq 1.4R$. This inequality establishes the range of applicability of boundary homogenization in the external problem. For smaller values of R_{out} , the relative error increases as R_{out} decreases, that is not surprising since this range of the outside radius is beyond the scope of applicability of the boundary homogenization approach.

IV. CONCLUDING REMARKS

This study is devoted to trapping of diffusing particles by periodically striped, cylindrical surfaces. Its main idea is that one can replace non-uniform boundary conditions on the surface by an effective uniform partially absorbing boundary condition with the effective trapping rate κ_{eff} given by Eq. (1.2). Such a replacement, called boundary homogenization, reduces the initial three-dimensional problem with non-uniform boundary conditions to an effective one-dimensional one, which can be readily solved analytically, as discussed in Sec. II and in the Appendix. Although initially the expression for the effective trapping rate in Eq. (1.2) was obtained for flat surfaces, our analysis above shows that this expression “works” very well for cylindrical surfaces also.

While the main focus of this study is on the mean particle lifetime, one might expect that boundary homogenization can be successfully used to find higher moments of the lifetime, as well as the particle survival probability, $S(t)$, and the lifetime probability density, $\varphi(t) = -dS(t)/dt$. In Fig. 6, we present $S(t)$ and $\varphi(t)$ obtained from the simulations (symbols) of the internal problem in the same cylindrical tube of radius $R = L/\pi$, with the stripe surface fraction $\sigma = l/L = 0.2$, for two different stripe orientations, perpendicular and parallel ($n = 2$) to the tube axis. In all simulations, the particle initial distribution inside the tube was uniform. The solid curves in this figure are numerically inverted Laplace transforms of $S(t)$ and $\varphi(t)$. These Laplace transforms, denoted by $\hat{S}(s)$ and $\hat{\varphi}(s)$, are derived in the Appendix. As shown in the Appendix, these Laplace transforms are given by

$$\hat{S}(s) = \frac{1}{s} (1 - \hat{\varphi}(s)) \quad (4.1)$$

and

$$\hat{\varphi}(s) = \frac{2\kappa_{\text{eff}}\sqrt{D}I_1(R\sqrt{s/D})}{R\sqrt{s}[\kappa_{\text{eff}}I_0(R\sqrt{s/D}) + \sqrt{sD}I_1(R\sqrt{s/D})]}, \quad (4.2)$$

where $I_0(z)$ and $I_1(z)$ are the modified Bessel functions.³³ One can see that all symbols fall on the same theoretical curves which are universal in the sense that they are independent of the stripe orientation.

Based on the above analysis, we hypothesize that the effective trapping rate κ_{eff} in Eq. (1.2) is an intrinsic property of the periodically striped surface. Therefore, the boundary homogenization approach to the description of trapping of diffusing particles by such surfaces is applicable not only for the three specific stripe orientations with respect to the tube axis, discussed above, but also for an arbitrary orientation. This is one of the main conclusions of this work.

While here we analyze trapping of diffusing particles, similar problems arise in other fields such as electrostatics and hydrodynamics. For example, several groups studied the

FIG. 6. The particle lifetime probability density $\varphi(t)$ and its survival probability $S(t)$ (inset) obtained from the simulations of the internal problem in the same cylindrical tube of radius $R = L/\pi$, with the stripe surface fraction $\sigma = l/L = 0.2$, for two different stripe orientations, perpendicular and parallel ($n = 2$) to the tube axis, and predicted by the theory using boundary homogenization. Symbols are the simulation results for perpendicular (circles) and parallel (squares) stripe orientations with respect to the tube axis, and solid curves are the theoretical dependences obtained by numerically inverting the Laplace transforms of $\hat{S}(s)$ and $\hat{\varphi}(s)$ given by Eqs. (4.1) and (4.2).

Poiseuille flow over periodic flat and cylindrical surfaces containing alternating stripes of two different materials with no-slip and no no-shear boundary conditions,^{31,34–39} which correspond to absorbing and reflecting boundary conditions in the case of diffusing particles, respectively. Although the problems of the Poiseuille flow and trapping of diffusing particles are similar, there is a fundamental difference between the two. The latter deals with a scalar quantity, concentration of diffusing particles. Its analog in the case of Poiseuille flow is the density of the fluid momentum in the flow direction. As a consequence, the results for the flow over a striped surface depend on the stripe orientation with respect to the flow direction, while for trapping of diffusing particles, the results are independent of the stripe direction. Analytical results for the flow over a striped surface also can be interpreted in terms of an effective uniform boundary condition for the velocity field on the surface.^{37,38} In the case of stripes parallel to the flow this boundary condition, reformulated in terms of effective trapping rate for diffusing particles leads to the expression for κ_{eff} , which is identical to that in Eq. (1.2).

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APPENDIX: PROBABILITY DENSITY OF THE PARTICLE LIFETIME IN A DISK WITH PARTIALLY ABSORBING BOUNDARY

Consider a particle diffusing in a circular disk with partially absorbing boundary. At $t = 0$, the particle starting point is uniformly distributed over the disk area. To simplify the notations, here we assume that the disk radius and the diffusion constant are equal to unity, $R = D = 1$. The probability density $p(r, t)$ of finding the particle at point $\mathbf{r}$, $r = |\mathbf{r}|$, at time t satisfies

$$\frac{\partial p}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial p}{\partial r} \right), \quad r \leq 1, \quad (A1)$$

subject to the initial condition $p(r, 0) = 1/\pi$ and boundary conditions

$$\left. \frac{\partial p}{\partial r} \right|_{r=0} = 0, \quad - \left. \frac{\partial p}{\partial r} \right|_{r=1} = \kappa p(1, t). \quad (A2)$$

The Laplace transform of $p(r, t)$, denoted by $\hat{p}(r, s)$ ($\hat{p}(r, s) = \int_0^\infty e^{-st} p(r, t) dt$), satisfies

$$s\hat{p} - \frac{1}{\pi} = \frac{d^2\hat{p}}{dr^2} + \frac{1}{r} \frac{d\hat{p}}{dr}, \quad r \leq 1. \quad (\text{A3})$$

It is convenient to introduce function $w(r, s) = \hat{p}(r, s) - 1/(\pi s)$, which satisfies

$$\frac{d^2w}{dr^2} + \frac{1}{r} \frac{dw}{dr} - sw = 0, \quad r \leq 1. \quad (\text{A4})$$

A general solution for $w(r, s)$ is given by

$$w(r, s) = aI_0(r\sqrt{s}) + bK_0(r\sqrt{s}), \quad (\text{A5})$$

where $I_n(z)$ and $K_n(z)$ are the modified Bessel functions.³³ Factors a and b can be determined from the boundary conditions in Eq. (A2). Using the relations $dI_0(z)/dz = I_1(z)$ and $dK_0(z)/dz = -K_1(z)$,³³ we obtain $b = 0$ and

$$a = -\frac{\kappa}{\pi s [\kappa I_0(\sqrt{s}) + \sqrt{s} I_1(\sqrt{s})]}. \quad (\text{A6})$$

Thus, the Laplace transform of the probability density is given by

$$\hat{p}(r, s) = aI_0(r\sqrt{s}) + \frac{1}{\pi s}. \quad (\text{A7})$$

The particle lifetime probability density $\varphi(t)$ is related to the probability density $p(r, t)$ by the relation $\varphi(t) = 2\pi\kappa p(1, t)$. Using this together with Eqs. (A6) and (A7), we find the Laplace transform of $\varphi(t)$, denoted by $\hat{\varphi}(s)$,

$$\hat{\varphi}(s) = 2\pi\kappa\hat{p}(\sqrt{s}) = \frac{2\kappa I_1(\sqrt{s})}{\sqrt{s} [\kappa I_0(\sqrt{s}) + \sqrt{s} I_1(\sqrt{s})]}. \quad (\text{A8})$$

To obtain the expression for the Laplace transform of the lifetime probability density when the disk radius and the diffusion constant are not equal to unity, one has to replace here κ by $\kappa_{\text{eff}}R/D$ and s by sR^2/D . This leads to the expression for $\hat{\varphi}(s)$ given in Eq. (4.2) of the main text.

The particle survival probability, $S(t)$, and the lifetime probability density $\varphi(t)$ are related by the relation

$$\varphi(t) = -\frac{dS(t)}{dt}. \quad (\text{A9})$$

After the Laplace transformation, this relation takes the form

$$\hat{\varphi}(s) = -s\hat{S}(s) + 1, \quad (\text{A10})$$

where $\hat{S}(s)$ is the Laplace transform of the survival probability $S(t)$. Solving Eq. (A10) with respect to $\hat{S}(s)$, we arrive at Eq. (4.1) from the main text.

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