Note: Boundary homogenization for a circle with periodic absorbing arcs. Exact expression for the effective trapping rate

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Trapping of diffusing particles by absorbing regions on the otherwise reflecting surface plays an important role in different technological and biophysical processes such as electric current through an array of microelectrodes,¹ reactions on supported catalysts,² transport through porous membranes,³ water exchange in plants,⁴ ligand binding to cell surface receptors,⁵ ligand accumulation in cell culture assays.⁶ Such trapping problems are notoriously difficult for analytical treatment because of the heterogeneous boundary conditions on the surface. Recently, we managed to overcome this difficulty and develop an approximate analytical theory of trapping in the special case of cylindrical surfaces with periodic absorbing stripes.⁷ Comparison showed that the mean particle lifetime predicted theoretically agrees well with its counterpart obtained from Brownian dynamics simulations. The comparison was made at three orientations of the stripes with respect to the cylinder axis (parallel, perpendicular, and at the angle $\pi/4$ to the axis) for both internal and external problems, where the particles diffused inside and outside the cylinder, respectively.

The theory was developed using an approximate approach called boundary homogenization (BH).^{8,9} Its main idea is to replace the heterogeneous boundary conditions on the surface by a homogeneous one with a properly chosen effective trapping rate. This is possible because, due to diffusion, the “memory” of the shape and size of the absorbing regions, their concentration and arrangement on the boundary decays with the distance from the boundary. At sufficiently large distances, the steady-state particle fluxes and concentrations are indistinguishable from their counterparts in the case of a uniform partially absorbing boundary with a properly chosen surface trapping rate. This trapping rate, denoted by κ , is the key quantity which one needs to know to study trapping by a heterogeneous boundary in the framework of the BH approach.

Finding an analytical expression for κ is an extremely difficult task. In our analysis of trapping by striped cylindrical surfaces,⁷ we took advantage of the known exact expression for κ for periodically striped flat surfaces.⁹ We applied this expression to cylindrical surfaces formed by rolling corresponding flat surfaces. It has been found that the expression also works well for cylindrical geometry. Moreover, when the stripes are parallel to the cylinder axis, BH

leads to the known exact result for the mean particle lifetime in the internal problem with uniform initial distribution of the particle starting point. This exact result was recently obtained by Rupprecht *et al.*¹⁰ from a rather complicated exact solution for the particle survival probability as a function of time and the particle starting point, which they derived. The fact that BH leads to the exact result for the mean particle lifetime suggests that the exact expression for the effective trapping rate of a flat periodically striped surface remains exact in the cylindrical geometry with the stripes parallel to the cylinder axis. The aim of this note is to prove this suggestion.

When the stripes are parallel to the cylinder axis, the system is invariant with respect to translations in the direction of the axis, and the trapping problem in such a system is, in fact, two-dimensional. Therefore, in the rest of this note, we study trapping of particles diffusing on a flat surface by a circle of radius R whose boundary contains n identical, evenly spaced absorbing arcs of length l , separated by reflecting arcs of length $L - l$, where the period L of the system is related to the circle radius by the relation $L = 2\pi R/n$, $n = 1, 2, 3, \dots$. In such a circle, the absorbing arcs occupy the fraction $\sigma = l/L = nl/(2\pi R)$ of its boundary, $0 \leq \sigma \leq 1$.

Consider steady-state trapping of particles diffusing in an annulus bounded by the outer circle of radius R , with alternating absorbing and reflecting arcs mentioned above and an inner circle of radius a , where the particle concentration c_a is kept constant. The BH approach is applicable when a is small compared to R . In such a case, the outer circle may be considered as a uniform partially absorbing boundary, characterized by an effective trapping rate, denoted by κ_c . Then the steady-state particle concentration $c(r)$ inside the annulus is independent of the angle and satisfies

$$-2\pi D r \frac{dc(r)}{dr} = J, \quad a < r < R, \quad (1)$$

where D is the particle diffusivity and J is the total steady-state flux. Solving this equation with the boundary conditions,

$$c(a) = c_a, \quad 2\pi R \kappa_c c(R) = J, \quad (2)$$

one can find the concentration profile $c(r)$ and the total flux J .

We can map the annulus in the polar coordinates r and φ , $a \leq r \leq R$, $0 \leq \varphi \leq 2\pi$, onto a rectangle in the xy plane using the coordinate transformation,

$$x(r, \varphi) = R\varphi, \quad y(r, \varphi) = -R \ln(R/r). \quad (3)$$

This transformation straightens the outer circle without changing its length and converts the annulus into a rectangle of length $2\pi R$, $0 \leq x \leq 2\pi R$, and width $R \ln(R/a)$, $-R \ln(R/a) \leq y \leq 0$. After the transformation, Eq. (1) reduces to

$$-2\pi R D \frac{dc(y)}{dy} = J, \quad -R \ln(R/a) < y < 0, \quad (4)$$

and the boundary conditions in Eq. (2) take the form

$$c(y)|_{y=-R \ln(R/a)} = c_a, \quad 2\pi R \kappa_c c(y)|_{y=0} = J. \quad (5)$$

The two equations above describe the uniform steady-state concentration profile $c(y)$ in the rectangle with reflecting boundaries at $x = 0$ and $x = 2\pi R$ in the presence of a uniform flux between the lower and upper boundaries of the rectangle, located at $y = -R \ln(R/a)$ and $y = 0$, respectively. The uniform flux density j is given by

$$j = \frac{J}{2\pi R} = \kappa_c c(y)|_{y=0} = -D \frac{dc(y)}{dy}. \quad (6)$$

Applying the coordinate transformation in Eq. (3) to the initial problem of trapping of diffusing particles by the outer circle of the annulus with alternating absorbing and reflecting arcs, we map this problem onto the trapping problem in the rectangle, whose upper boundary is the straightened outer circle. When the radius a is sufficiently small, the width of the rectangle, $R \ln(R/a)$, is large enough, so that BH can be used to analyze trapping in the rectangle whose upper boundary contains alternating absorbing and reflecting intervals of length l and $L - l$. The effective trapping rate of the rectangle boundary, denoted by κ_r , is identical to the effective trapping rate κ of a flat periodically striped surface of period L with absorbing stripes of length l . Using the exact expression for κ ,⁹ we arrive at

$$\kappa_r = \kappa = \frac{\pi D}{L \ln[1/\sin(\pi\sigma/2)]}, \quad \sigma = \frac{l}{L} = \frac{nl}{2\pi R}. \quad (7)$$

The steady-state flux density in the rectangle is just the steady-state flux density in Eq. (6), in which κ_c replaced by κ_r . Since the two flux densities are equal, the two trapping rates are also equal, $\kappa_c = \kappa_r$, and Eq. (7) provides an exact expression for κ_c . Finally, we use Eq. (7) and the relation $L = 2\pi R/n$ to write the effective trapping rate κ_c in terms of the outer circle radius R , the number n of the absorbing arcs, and their line fraction $\sigma = l/L = nl/(2\pi R)$ as

$$\kappa_c = \frac{nD}{2R \ln[1/\sin(\pi\sigma/2)]}. \quad (8)$$

This is the main result of this note. Although the focus of the above discussion is on the internal problem, similar consideration can be applied to the external problem, leading to the same expression for κ_c in Eq. (8).

It is worth noting that the identity of the trapping rates, $\kappa_c = \kappa_r$, can also be proved by using the invariance of the underlying Laplace equation and alternating absorbing-reflecting boundary conditions under conformal mapping, which preserves the total flux across the boundary (see Ref. 11 and references therein). The coordinate transformation in Eq. (3) is an example of such a mapping.¹²

Finally, we note that although the above analysis and that in Ref. 7 focus on the steady-state flux and the mean particle lifetime, respectively, BH can also be used to find higher moments of the particle lifetime, the lifetime probability density, $\varphi(t)$, and the particle survival probability, $S(t)$. As demonstrated in Ref. 7, functions $\varphi(t)$ and $S(t)$ predicted theoretically using BH are in perfect agreement with the values of these functions obtained from Brownian dynamics simulations. However, we do not have a rigorous proof that BH provides an exact solution for these functions and for the higher moments of the particle lifetime.

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