Steady-state flux of diffusing particles to a rough boundary formed by absorbing spikes periodically protruding from a reflecting base

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ABSTRACT

We study steady-state flux of particles diffusing on a flat surface and trapped by absorbing spikes of arbitrary length periodically protruding from a reflecting base. It is assumed that the particle concentration, far from this comblike boundary, is kept constant. To find the flux, we use a boundary regularization approach that replaces the initial highly rough and heterogeneous boundary by an effective boundary which is smooth and uniform. After such a replacement, the two-dimensional diffusion problem becomes essentially one-dimensional, and the steady-state flux can be readily found. Our main results are simple analytical expressions determining the position of the smooth effective boundary and its uniform trapping rate as functions of the spike length and interspike distance. It is shown that the steady-state flux to the effective boundary is identical to its counterpart to the initial boundary at large distances from this boundary. Our analytical results are corroborated by Brownian dynamics simulations.

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I. INTRODUCTION

The classical Smoluchowski-Collins-Kimball theory describes trapping of diffusing particles by smooth, uniformly absorbing surfaces. However, researchers frequently have to deal with trapping by rough heterogeneous surfaces. These problems are notoriously difficult for analytical treatment because of the geometric complexity of the boundaries and nonuniformity of the boundary conditions. Examples of such problems include transport through porous membranes, ligand binding to cell surface receptors, heterogeneous catalysis, electric current through microelectrodes, sensing systems, smart antibacterial coatings, tracer dispersion in global geophysical systems (atmosphere, ocean, and geological media), and diffusion-limited needle aggregation (see Refs. 1–16 and references therein). Note that conceptually similar difficulties arise in other areas such as hydrodynamics, electrostatics, heat transfer, and surface wettability (see Refs. 17–34 and references therein).

In this paper, we show how to overcome these difficulties in two dimensions by developing an analytical theory of trapping of diffusing particles by rough, heterogeneous boundaries in the special case where these boundaries are formed by absorbing spikes of arbitrary height, periodically protruding from a reflecting base, as shown in panels (a) and (c) of Fig. 1. To be more specific, we study the two-dimensional steady-state flux to such a comblike boundary, on condition that the particle concentration sufficiently far from the boundary is kept constant. Our approach to the problem is based on the observation that the effect of the boundary structure on the flux decreases with the distance from the boundary. As this distance increases, the flux loses memory about the boundary structure. The lateral component of the flux vanishes, and it becomes essentially one-dimensional, directed normal to the boundary.

We have used this observation earlier to homogenize boundary conditions on smooth heterogeneous boundaries,^{35–41} i.e., to

FIG. 1. Schematic representation of a strip of width L with perfectly absorbing spikes of height H periodically, with period W , protruding from the reflecting base. The particle concentration at the upper strip boundary is kept constant and equal to C_L . Panels (a) and (c) show long and short spikes. In panels (b) and (d), the effective absorbing boundaries are shown by bold solid lines, while the dashed lines show the spike heights. The displacement Δ of the effective perfectly absorbing boundary from the reflecting base is positive for long spikes and negative for short spikes, as shown in panels (b) and (d), respectively.

approximately replace the initial boundary conditions by a homogeneous one chosen so as to accurately predict the steady-state flux to the boundary. Recently, this observation was applied to smoothing rough uniformly absorbing boundaries.^{42–44} In Ref. 42, Skvortsov and Walker considered trapping of particles diffusing on a surface toward a rough boundary formed by absorbing spikes periodically protruding from an absorbing base. They showed that this boundary absorbs the particles equivalently to a smooth absorbing boundary elevated above the base and derived an expression for the elevation height, Δ ,

$$\Delta = \frac{W}{\pi} \ln \left[\frac{1}{\cosh(\pi H/W)} \right], \quad (1.1)$$

where H and W are the spike height and interspike distance, respectively. In Ref. 43, this result was used to demonstrate that a rough absorber formed by absorbing spikes periodically protruding from an absorbing circular core can be replaced by a smooth circular absorber with a properly chosen effective radius.

Conceptually, both boundary homogenization and smoothing can be considered as special cases of a general approach that can be termed boundary regularization, but there is an important difference between the two. In smoothing of an absorbing rough boundary, the goal is to find the location of the effective smooth absorbing boundary. In homogenization of a smooth boundary, the effective boundary location remains unchanged while heterogeneous boundary conditions on this boundary are replaced by an effective homogeneous boundary condition which is the radiation boundary condition with a properly chosen trapping rate. Here, we study trapping by the boundary which is both rough and heterogeneous. In this case, regularization of the boundary may include both its homogenization and displacement. The limiting case of short absorbing spikes, $H \ll W$, periodically protruding from a reflecting base has recently

been considered in Ref. 44. It was shown that when the spikes are short, the effective boundary is partially absorbing and coincides with the base. The effective trapping rate, κ , in this case is given by

$$\kappa = \frac{\pi D}{W \ln[1/\sin(\pi H/W)]}, \quad (1.2)$$

where D is the particle diffusivity. This trapping rate characterizes the boundary trapping efficiency, and $\kappa = 0$ and $\kappa = \infty$ correspond to perfectly reflecting and absorbing boundaries, respectively.

The outline of this paper is as follows: In Sec. II, we state the problem and discuss our main results, including their numerical test in Brownian dynamics simulations. Derivation of these results is given in Sec. III. Some concluding remarks are made in Sec. IV.

II. MAIN RESULT

Consider point particles diffusing, with the diffusivity D , in a two-dimensional strip of width L , $0 < y < L$. The lower strip boundary has a comblike structure formed by infinitely thin absorbing spikes of height H periodically, with period W , protruding from a reflecting base located at $y = 0$ [see panels (a) and (c) of Fig. 1]. The particle concentration at the upper boundary, located at $y = L$, is kept constant and equal to C_L so that the system of diffusing particles is in steady state. Our focus is on the steady-state flux of these particles to the comblike boundary. If this boundary is flat (no spikes) and partially absorbing, with the trapping rate κ , the problem is one-dimensional, the flux is directed along the y -axis, and its density, j_κ , is given by

$$j_\kappa = \frac{D}{L + D/\kappa} C_L. \quad (2.1)$$

In the limiting case of perfectly absorbing boundary ($\kappa = \infty$), Eq. (2.1) simplifies and reduces to

$$j_\infty = \frac{D}{L} C_L. \quad (2.2)$$

In the case of a comblike boundary, the flux near the boundary is rather complicated. However, when L is large enough, $L \gg H, W$, the flux, sufficiently far from the boundary, is essentially one-dimensional and directed along the y -axis. Our goal is to find how the asymptotic behavior of the flux density, denoted by j , depends on the boundary geometric parameters, H and W .

As derived in Sec. III, this asymptotic behavior is given by

$$j = \begin{cases} \frac{D}{L - \Delta} C_L, & H \geq H^* \\ \frac{D}{L + D/\kappa} C_L, & H \leq H^*, \end{cases} \quad (2.3)$$

where $H^* = (W/\pi) \ln(1 + \sqrt{2})$ is the critical value of the spike height that separates the two regimes, and the parameters Δ and κ are

$$\Delta = (W/\pi) \ln[\sinh(\pi H/W)], \quad (2.4)$$

$$\kappa = \frac{D}{|\Delta|} = \frac{\pi D}{W \ln[1/\sinh(\pi H/W)]}. \quad (2.5)$$

Parameter Δ indicates the position of an effective perfectly absorbing boundary, counted from the reflecting base, and hence separated from the upper strip boundary by the distance $L - \Delta$. When spikes are long enough, $H \geq H^*$, Δ is non-negative, and the flux in Eq. (2.3) is identical to its counterpart to the flat perfectly absorbing boundary located at distance Δ above the reflecting base [see Fig. 1(b)]. For shorter spikes, whose height satisfies the inequality $H < H^*$, Δ is negative, and the effective flat perfectly absorbing boundary is located below the reflecting base [see Fig. 1(d)]. In this case, the flux in Eq. (2.3) is identical to its counterpart to the partially absorbing boundary located at $y = 0$, which is characterized by the trapping rate κ given in Eq. (2.5). To summarize, the flux in Eq. (2.3) is identical to the flux to the effective flat boundary whose location Δ_{eff} and trapping rate κ_{eff} are

$$\Delta_{\text{eff}} = \begin{cases} \Delta = (W/\pi) \ln[\sinh(\pi H/W)], & H \geq H^* \\ 0, & H < H^*, \end{cases} \quad (2.6)$$

$$\kappa_{\text{eff}} = \begin{cases} \infty, & H \geq H^* \\ (D/|\Delta|) = \pi D / \{W \ln[1/\sinh(\pi H/W)]\}, & H < H^*. \end{cases} \quad (2.7)$$

These dependences are illustrated in Fig. 2.

For long spikes, $H \gg W$, Δ_{eff} in Eq. (2.6) reduces to

$$\Delta_{\text{eff}} = H - (W/\pi) \ln 2, \quad (2.8)$$

which coincides with the location of the effective flat absorbing boundary given by Eq. (1.1), at $H \gg W$. This should be expected. Indeed, the Skvortsov-Walker theory⁴² describes trapping by absorbing spikes periodically protruding from the absorbing base. When the spike height exceeds the boundary period, particles are trapped by the spikes before they reach the base. As a consequence, it does not matter whether the base is reflecting or absorbing.

As the spike height tends to zero, the effective surface trapping rate, κ_{eff} , vanishes. Formally, this happens because, as follows from

FIG. 2. Position of the effective boundary, Δ_{eff} [Eq. (2.6)] (blue line), and its trapping rate, κ_{eff} [Eq. (2.7)] (red line), as functions of the of the geometric parameters, the spike height, H , and the interspike distance, W . The spike height, $H/W = \pi^{-1} \ln(1 + \sqrt{2})$, separates short and long spikes.

Eq. (2.4), the position of the effective absorbing boundary goes to minus infinity, as $H/W \rightarrow 0$. According to Eq. (2.7), the limiting behavior of κ_{eff} in this case is

$$\kappa_{\text{eff}} = \pi D / \{W \ln[W/(\pi H)]\}, \quad (2.9)$$

which agrees with the limiting behavior of κ in Eq. (1.2) given by the theory developed for short spikes.⁴⁴

A. Numerical test

To check the accuracy of the obtained results, we determine the location of the effective perfectly absorbing flat boundary in Brownian dynamics simulations and compare the boundary position Δ obtained from the simulations with that given by Eq. (2.4). In simulations, we find the mean particle lifetime, τ_{sim} , for the uniform distribution of the particle starting point over the line $y = H$. The mean lifetime of such a particle in the presence of a perfectly absorbing boundary located at $y = \Delta$, denoted by τ_{Δ} , is

$$\tau_{\Delta} = \frac{(H - \Delta)(2L - \Delta - H)}{2D}. \quad (2.10)$$

Assuming that $\tau_{\text{sim}} = \tau_{\Delta}$, we use τ_{sim} to find Δ by solving Eq. (2.10). The result is

$$\Delta = L - \sqrt{2D\tau_{\text{sim}} + (L - H)^2}. \quad (2.11)$$

The theoretical dependence of Δ on H and W [Eq. (2.4)] is compared with the simulation results in Fig. 3. In Fig. 3, the theoretical dependence is shown by the solid line and the symbols show the values of the ratio Δ/W for spikes of different heights, $H/W = 0.05, 0.1, 0.5, 1.0, 1.5, 2.0, 2.5$, and 3.0 , obtained in simulations with $L = H + 5W$. One can see excellent agreement between the theoretical predictions and the simulation results.

FIG. 3. Position of the effective perfectly absorbing boundary, Δ , as a function of the spike height, H , and the interspike distance, W . The solid line shows the theoretically predicted dependence [Eq. (2.4)] $\Delta/W = (1/\pi) \ln[\sinh(\pi H/W)]$. Symbols are boundary positions obtained in Brownian dynamics simulations for spikes of different heights: $H/W = 0.05, 0.1, 0.5, 1.0, 1.5, 2.0, 2.5$, and 3.0 . The simulations were performed for the strips of width $L = H + 5W$. The vertical dashed line at $H/W = \pi^{-1} \ln(1 + \sqrt{2})$ corresponds to the boundary separating short and long spikes.

III. DERIVATION

In this section, we derive the expression for the steady-state flux density to the comblike boundary [see panels (a) and (c) of Fig. 1] sufficiently far from this boundary [Eqs. (2.3)–(2.5)], assuming that the strip width is large enough, $L \gg H, W$. Specifically, we show that the steady-state concentration approaches its upper limit C_L as if there is a uniform perfectly absorbing boundary located at distance $|\Delta|$ above (below) the base when $\Delta > 0$ ($\Delta < 0$), where Δ is given in Eq. (2.4). When $\Delta = 0$, this boundary coincides with the base. The above-mentioned result for the position of the effective boundary is used to find the steady-state flux. The effective boundary position is obtained by means of the method of conformal mapping, which is not frequently used in studies of diffusion-influenced kinetics. Therefore, all steps of the derivation are discussed in detail. One can find a discussion of the method of conformal mapping and its numerous applications in many textbooks on functions of complex variables (see, for example, Refs. 45–47).

It is convenient to rescale the initial coordinates by the factor π/W and to use dimensionless coordinates x and y , in which the boundary period, i.e., the distance between neighboring spikes, is π , the dimensionless spike height and strip width are $h = \pi H/W$ and $l = \pi L/W$, respectively. It will be assumed that the spikes are located at $x = n\pi + \pi/2$, $n = 0, \pm 1, \pm 2, \dots$. Taking advantage of the system symmetry, we calculate the steady-state flux density in the rectangle, $-\pi/2 \leq x \leq \pi/2$, $0 \leq y \leq l$, which forms one strip period [see Fig. 4(a)]. The steady-state particle concentration, $C(x, y)$, in the rectangle satisfies the Laplace equation

$$\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} = 0, \quad (3.1)$$

subject to the absorbing boundary conditions on the spikes, $x = \pm\pi/2$, $0 \leq y \leq h$, and the reflecting boundary condition on the rest of the rectangle boundary, except its upper part, $-\pi/2 \leq x \leq \pi/2$, $y = l$, where the concentration is kept constant, $C = C_{\max}$.

Consider a coordinate transformation (map)

$$u = u(x, y), \quad v = v(x, y). \quad (3.2)$$

When the real-valued functions $u(x, y)$ and $v(x, y)$ satisfy the Cauchy-Riemann equations,

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \quad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}, \quad (3.3)$$

the concentration, considered as a function of u and v , $C(u, v) = C(u(x, y), v(x, y))$, is also a solution of the Laplace equation

$$\frac{\partial^2 C}{\partial u^2} + \frac{\partial^2 C}{\partial v^2} = 0. \quad (3.4)$$

If we consider the coordinates x and y as the real and imaginary parts of a complex variable z , $z = x + iy$, where $i = \sqrt{-1}$, and u and v as the real and imaginary parts of a complex variable w , $w = u + iv$, then the coordinate transformation in Eq. (3.2) is a conformal map of the complex z -plane onto the complex w -plane, $w(z) = u(z) + iv(z)$.

As we will see, there is a conformal map, $w(z)$,

$$w(z) = \arcsin[\sin(z)/\cosh(h)], \quad (3.5)$$

which converts the Laplace equation for $C(x, y)$ in the z -plane with inconvenient boundary conditions discussed above to the same equation for $C(u, v)$ in the w -plane with much simpler boundary conditions [see Fig. 4(b)], which allow for an exact solution for $C(u, v)$ sufficiently far from the lower heterogeneous boundary. Below we consider how the initial rectangle [Fig. 4(a)] is transformed under a sequence of the three transformations resulting in $w(z)$ in Eq. (3.5). Each of these transformations is a conformal map. Therefore, the Laplace equation remains unchanged under these transformations.

We begin with the transformation $w_1(z) = \sin(z)$,

$$\begin{aligned} w_1(z) = \sin(z) &= \sin(x) \cosh(y) + i \cosh(x) \sin(y) \\ &= u_1(z) + iv_1(z). \end{aligned} \quad (3.6)$$

FIG. 4. Transformation of the rectangle in the complex z -plane ($z = x + iy$) under conformal mapping of the z -plane onto the w -plane [$w(z) = u(z) + iv(z)$]. Panel (a) shows the initial rectangle in the z -plane, which contains absorbing intervals (spikes) on its vertical sides. Here, l is the y -coordinate of the rectangle upper boundary, where the particle concentration is kept constant, $l = \pi L/W$. Panel (b) shows the rectangle in the w -plane obtained by conformal mapping, $w(z) = \arcsin[\sin(z)/\cosh(h)]$, of the initial rectangle, where $h = \pi H/W$. Here, l' is the v -coordinate of the rectangle upper boundary, given in Eq. (3.11). As a result of conformal mapping, the absorbing intervals moved from the vertical sides of the initial rectangle to the bottom side of the rectangle in the w -plane. This allows for homogenization of the heterogeneous boundary conditions on the bottom side, as illustrated in panel (c).

This transformation maps the infinite strip in the z -plane, $-\pi/2 \leq x \leq \pi/2$, $y \geq 0$, onto the upper half plane, $v_1 \geq 0$, in the w_1 -plane. It maps the six points shown in Fig. 4(a), which determine the system geometry, $z_1 = -\pi/2 + ih$, $z_2 = -\pi/2$, $z_3 = \pi/2$, $z_4 = \pi/2 + ih$, $z_5 = -\pi/2 + il$, and $z_6 = \pi/2 + il$, to the following points in the w_1 -plane: $w_1(z_1) = -\cosh(h)$, $w_1(z_2) = -1$, $w_1(z_3) = 1$, $w_1(z_4) = \cosh(h)$, $w_1(z_5) = -\cosh(l)$, and $w_1(z_6) = \cosh(l)$. The upper boundary of the rectangle in the z -plane, $z = x + il$, $-\pi/2 \leq x \leq \pi/2$, becomes the top half of the ellipse in the w_1 -plane given by

$$\left(\frac{u_1}{\cosh(l)}\right)^2 + \left(\frac{v_1}{\sinh(l)}\right)^2 = 1, \quad v_1 \geq 0. \quad (3.7)$$

Next, we apply the uniform compression transformation

$$w_2(z) = \frac{w_1(z)}{\cosh(h)} = u_2(z) + iv_2(z), \quad (3.8)$$

which maps the spike top and bottom points [see Fig. 4(a)] to points $w_2(z_1) = -1$, $w_2(z_4) = 1$ and $w_2(z_2) = -1/\cosh(h)$, $w_2(z_3) = 1/\cosh(h)$ in the w_2 -plane, respectively. Points 5 and 6 are transformed to points $w_2(z_5) = -\cosh(l)/\cosh(h)$ and $w_2(z_6) = \cosh(l)/\cosh(h)$, and the upper boundary of the rectangle is transformed into the top half of the ellipse obtained by compression of the ellipse in Eq. (3.7),

$$\left(\frac{u_2}{\cosh(l)}\right)^2 + \left(\frac{v_2}{\sinh(l)}\right)^2 = \frac{1}{(\cosh(h))^2}, \quad v_2 \geq 0. \quad (3.9)$$

Finally, we apply the last transformation

$$w(z) = \arcsin(w_2(z)) = u(z) + iv(z) \quad (3.10)$$

that converts the upper half plane, $v_2 \geq 0$, in the w_2 -plane into an infinite strip, $-\pi/2 \leq u \leq \pi/2$, $v \geq 0$, in the w -plane. This transformation converts the top half of the ellipse, given in Eq. (3.9), in the w_2 -plane into the upper boundary of the rectangle of width l' in the w -plane, $-\pi/2 \leq u \leq \pi/2$, $v = l'$. Coordinates of points 1–6, in this plane, are $w(z_1) = -\pi/2$, $w(z_2) = -\arcsin(1/\cosh(h))$, $w(z_3) = \arcsin(1/\cosh(h))$, $w(z_4) = \pi/2$, $w(z_5) = -\pi/2 + il'$, $w(z_6) = \pi/2 + il'$. When the strip is wide enough, the rectangle width l' is given by (see Appendix A)

$$l' = \text{Im}\{\arcsin[\cosh(l)/\cosh(h)]\} \approx l - \ln(\cosh(h)). \quad (3.11)$$

Thus, the sequence of transformations discussed above converts the initial rectangle shown in panel (a) of Fig. 4 into the rectangle shown in panel (b). The key difference between the two rectangles is that the former contains the absorbing intervals (spikes) on its vertical sides, while the latter contains the absorbing intervals on the horizontal bottom side. This makes it possible to homogenize the heterogeneous boundary conditions on this side, as illustrated in Fig. 4(c). After that the diffusion problem becomes essentially one-dimensional. This eventually allows us to find the position of the effective perfectly absorbing boundary and then the steady-state flux on condition that the initial strip is wide enough, $L \gg H$, W .

The effective trapping rate of diffusing particles by this homogenized boundary is given by the Moizhes-Muratov-Shvartsman (MMS) formula⁴⁸

$$\kappa_{MMS} = \frac{D'}{\ln[1/\sin(\pi\sigma/2)]}, \quad (3.12)$$

where D' is the particle diffusivity in the w -plane and σ is the fraction of the bottom side occupied by the absorbing intervals. Moizhes⁴⁹ derived the electrostatic equivalent of this formula more than six decades ago, which was adapted for use in trapping of diffusing particles by Muratov and Shvartsman.⁴⁸ In the case of the rectangle shown in Fig. 4(b), the surface fraction, σ , of the absorbing part of the bottom side is

$$\sigma = 1 - (2/\pi) \arcsin(1/\cosh(h)). \quad (3.13)$$

Substituting this into Eq. (3.12), we arrive at

$$\kappa_{MMS} = \frac{D'}{\ln[\coth(h)]}. \quad (3.14)$$

When l significantly exceeds h and unity (and hence $l' \gg 1$), we can find how the concentration $C(u, v)$ approaches its maximum value $C_{\max} = C(l')$, which is independent of u . To this end, we take advantage of boundary homogenization, which makes the diffusion problem essentially one-dimensional, and find $C(v)$ by solving the equation

$$j' = D' \frac{dC(v)}{dv} = \kappa_{MMS} C(0), \quad (3.15)$$

where j' is the steady-state flux. The solution is given by

$$C(v) = \frac{v + D'/\kappa_{MMS}}{l' + D'/\kappa_{MMS}} C_{\max} = \frac{v + \ln(\coth(h))}{l - \ln(\sinh(h))} C_{\max}, \quad (3.16)$$

where the relations in Eqs. (3.11) and (3.14) have been used.

According to Eq. (3.5) [or Eq. (3.10)], we have

$$v(z) = v(x + iy) = \text{Im}\{\arcsin[\sin(z)/\cosh(h)]\}. \quad (3.17)$$

At $y \gg 1$, this reduces to (see Appendix B)

$$v(z) \approx y - \ln(\cosh(h)). \quad (3.18)$$

Substituting Eq. (3.18) for $v(z)$ into Eq. (3.16), we arrive at the y -dependence of the concentration,

$$C(y) = \frac{y - \ln(\sinh(h))}{l - \ln(\sinh(h))} C_{\max}, \quad (3.19)$$

which shows that the concentration linearly increases with y from zero to its maximum value, $C_{\max}$, as y increases from $\ln(\sinh(h))$ to l . This implies that the effective perfectly absorbing boundary is located at $y = y_a$,

$$y_a = \ln(\sinh(h)). \quad (3.20)$$

Returning to the dimensional variables, we obtain

$$(W/\pi)y_a = (W/\pi) \ln(\sinh(\pi H/W)) = \Delta, \quad (3.21)$$

which is the effective absorbing boundary position given in Eq. (2.4).

When $\sinh(\pi H/W) > 1$ (long spikes, whose height satisfies $H > H^*$), $\Delta > 0$, and the effective absorbing boundary is elevated above the reflecting base. The steady-state flux in this case is given by

the upper expression in Eq. (2.3). In the opposite case of short spikes, $H < H^*$, the situation is different. Here, $\sinh(\pi H/W) < 1$, $\Delta < 0$, and the effective absorbing boundary is located below the reflecting base. As a consequence, the expression for the steady-state flux takes the form

$$j = \frac{D}{L + |\Delta|} C_L. \quad (3.22)$$

We can interpret this flux as that to a partially absorbing boundary which coincides with the base. To this end, we note that the steady-state concentration, $C(y)$, satisfies the equation

$$\frac{dC(y)}{dy} = j, \quad (3.23)$$

with the absorbing boundary condition at $y = \Delta$, $C(\Delta) = 0$. Its y -dependence is given by

$$C(y) = \frac{y + |\Delta|}{L + |\Delta|} C_L. \quad (3.24)$$

Using this concentration at $y = 0$ (which corresponds to the reflecting base), we can write the flux in terms of $C(0) = |\Delta|C_L/(L + |\Delta|)$ as

$$j = \frac{D}{|\Delta|} C(0) = \kappa C(0), \quad (3.25)$$

where κ as a function of H and W is given in Eq. (2.5). Equation (2.5) may be considered as a partially absorbing boundary condition at $y = 0$. With this in mind, we can interpret the comblike boundary with short absorbing spikes periodically protruding from the reflecting base as a partially absorbing flat boundary, located at $y = 0$, which is characterized by the effective trapping rate, κ , given by Eq. (2.5). Using κ , we can write the steady-state flux in Eq. (3.22) in the form given in the lower line in Eq. (2.3). Finally, we note that when the spike height is equal to H^* (the boundary height separating short and long spikes), the effective flat boundary coincides with the reflecting base and is perfectly absorbing.

IV. SUMMARY

In this paper, we show how to handle trapping of diffusing particles by highly rough and heterogeneous boundaries shown in Fig. 1. A distinctive feature of such trapping problems is that they are intractable by conventional methods based on solving partial differential equations subject to heterogeneous boundary conditions. In view of this circumstance, we apply the boundary regularization approach which replaces the initial complex boundary by an effective smooth, uniformly absorbing one, with a properly chosen boundary position and trapping rate. In the previous works, we applied this approach for homogenization of boundary conditions on smooth heterogeneous boundaries,^{35–41} where the effective boundary coincides with the initial boundary, and the goal was to find the effective uniform trapping rate. Recently, this approach was used for smoothing highly rough absorbing boundaries,^{42,43} where the effective smooth boundary was absorbing, and the goal was to find its position. Here, we analyze the case where both the position and trapping rate of the effective smooth uniform boundary should be determined since the initial boundary is highly rough and heterogeneous.

Specifically, we study the steady-state flux of particles diffusing on a plane and trapped by absorbing spikes of arbitrary height periodically protruding from a reflecting base. It is assumed that the particle concentration sufficiently far from this comblike boundary is kept constant. Our main results are simple expressions determining the position and uniform trapping rate of the effective boundary as functions of the spike height and interspike distance, given in Eqs. (2.6) and (2.7), and illustrated in Fig. 2. After boundary regularization, the diffusion problem becomes essentially one-dimensional so that one can use the effective boundary to calculate the steady-state flux density which is given in Eq. (2.3). It is shown that this flux density is identical to the exact flux density sufficiently far from the comblike boundary, where the flux loses memory about the boundary structure and becomes essentially one-dimensional. Our analytical results are corroborated by Brownian dynamics simulations.

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APPENDIX A: DERIVATION OF THE RELATION $l' \approx l - \ln(\cosh(h))$

We wish to find the imaginary part, Y , of a complex number $Z = X + iY$ that satisfies

$$\sin(Z) = \frac{\cosh(l)}{\cosh(h)}. \quad (A1)$$

As follows from the relation

$$\sin(Z) = \sin(X + iY) = \sin(X) \cosh(Y) + i \cos(X) \sinh(Y), \quad (A2)$$

the real and imaginary parts of Z are solutions to the following system of equations:

$$\cos(X) \sinh(Y) = 0, \quad (A3)$$

$$\sin(X) \cosh(Y) = \frac{\cosh(l)}{\cosh(h)}. \quad (A4)$$

The real part of Z , determined from Eq. (A3), is $X = \pi/2$. Substituting this into Eq. (A4), we find that the imaginary part of Z is given by

$$Y = \text{rccosh} \left[\frac{\cosh(l)}{\cosh(h)} \right]. \quad (A5)$$

When $l \gg 1$, we can write

$$\frac{\cosh(l)}{\cosh(h)} \approx \frac{1}{2} e^{l - \ln(\cosh(h))} \approx \cosh[l - \ln(\cosh(h))]. \quad (A6)$$

Substituting this into Eq. (A5), we arrive at

$$Y = \text{Im} \left\{ \arcsin \left[\frac{\cosh(l)}{\cosh(h)} \right] \right\} \approx l - \ln(\cosh(h)). \quad (A7)$$

This expression is given in Eq. (3.11).

APPENDIX B: DERIVATION OF THE RELATION

$$v(z) = y - \ln(\cosh(h))$$

We wish to find the asymptotic behavior of $v(z) = v(x + iy)$, defined in Eq. (3.17),

$$v(z) = v(x + iy) = \text{Im}\{\arcsin[\sin(z)/\cosh(h)]\}, \quad (\text{B1})$$

at $y \gg 1$. The ratio $\sin(z)/\cosh(h)$ is

$$\frac{\sin(z)}{\cosh(h)} = \frac{1}{2i \cosh(h)} (e^{ix-y} - e^{-ix+y}). \quad (\text{B2})$$

When $y \gg 1$, this ratio can be approximately written as

$$\left. \frac{\sin(z)}{\cosh(h)} \right|_{y \gg 1} \approx -\frac{1}{2i} e^{-i\{x+i[y-\ln(\cosh(h))]\}} \approx \sin\{x+i[y-\ln(\cosh(h))]\}. \quad (\text{B3})$$

Substituting this into Eq. (B1), we arrive at the approximate expression for $v(z)$ given in Eq. (3.18).

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