Trapping of diffusing particles by spiky absorbers

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(Received 29 October 2017; accepted 31 January 2018; published online 22 February 2018)

We study trapping of particles diffusing on a flat surface by complex-shaped absorbers formed by periodic absorbing spikes protruding from absorbing circular cores. It is shown that a spiky absorber can be replaced by an equivalent, from the trapping point of view, circular absorber of properly chosen radius. A simple expression for the effective absorber radius in terms of the geometric parameters of the spiky absorber (the number and length of the spikes and the core radius) is derived. To check its accuracy and to establish the range of its applicability, we run Brownian dynamics simulations and obtain the mean lifetimes of particles diffusing inside a reflecting circle with different spiky absorbers placed in its center. These mean lifetimes are then compared with their counterparts given by the theory for equivalent circular absorbers. There is an excellent agreement between the lifetimes obtained by the two methods when the radius of the reflecting circle is sufficiently large. <https://doi.org/10.1063/1.5011060>

I. INTRODUCTION

Theory of diffusion-limited reactions mainly focuses on trapping of diffusing particles by absorbers of simple shapes, while researchers and engineers often have to deal with trapping by complex-shaped absorbers. Examples include dendritic solidification of liquids and alloys,^{1,2} cluster growth and kinetic gelation,³ transport across irregular interfaces like electrodes,⁴ diffusion-limited aggregation^{5,6} and tumor growth,^{7,8} performance of chemical reactors,⁹ etc. The geometric complexity of the absorbing surface makes the trapping problem analytically intractable. This necessitates the development of approximate approaches. The boundary smoothing approach discussed in the present work is a step in this direction.

We study trapping of particles diffusing on a flat surface by complex-shaped absorbers, the generic shape of which is shown in Fig. 1(a). The absorber is formed by n , $n = 1, 2, 3, \dots$, identical infinitely thin periodic absorbing spikes of length h protruding from an absorbing core (c) of radius a_c . Examples of no-core absorbers with $n = 1, 2$, and 4 are shown in Fig. 1(b). It is convenient to introduce the absorber size b , $b = a_c + h$, [see Fig. 1(a)] which is equal to h for a no-core absorber and a_c for a no-spike absorber, i.e., a circular absorber of radius b . Using this size as a length scale, we can write the core radius in the form $a_c = \varepsilon b$, where the dimensionless parameter ε varies between zero (no-core absorber) and unity (no-spike absorber), $0 \leq \varepsilon \leq 1$. Thus, the absorber is characterized by its size b and two dimensionless parameters n and ε .

The main result of this paper is an expression for the radius of an effective circular absorber which is equivalent to the initial spiky absorber from the particle trapping point of view. This expression and its numerical test are discussed in Secs. II and III. A derivation of the expression is given in Sec. IV. Section V contains some concluding remarks.

II. MAIN RESULT

To characterize trapping by our complex-shaped absorber (see Fig. 1), we consider the steady-state flux of diffusing particles to it, on condition that the particle concentration at a very large distance from the absorber is constant. We place the absorber at the origin and impose the requirement that the particle concentration is constant on a circle of radius R , $R \gg b$. The flux field is rather complex near the absorber. As the distance from the absorber increases, this field simplifies, and at sufficiently large distances, it has only the radial component. As a consequence, at such distances, the flux is indistinguishable from that to an effective (eff) absorbing circle of radius a_{eff} , centered at the origin.

With our choice of b as the length scale, we can write a_{eff} as

$$a_{eff} = bF(n, \varepsilon), \quad (2.1)$$

where $F(n, \varepsilon)$ is a dimensionless function of two dimensionless arguments n and ε . The main result of this paper, which is derived in Sec. IV, is a simple expression for this function,

$$F(n, \varepsilon) = \left(\frac{1 + \varepsilon^n}{2} \right)^{2/n}. \quad (2.2)$$

As $n \rightarrow \infty$, $F(n, \varepsilon) \rightarrow 1$, and the effective trapping radius approaches the size b of the absorber, $a_{eff} = b$, independent of the core radius.

In the absence of the core, $a_c = \varepsilon = 0$, we have

$$F(n, 0) = \frac{1}{2^{2/n}}, \quad a_{eff} = \frac{b}{2^{2/n}}. \quad (2.3)$$

In the absence of spikes, $a_c = b$, $\varepsilon = F(n, \varepsilon = 1) = 1$, and Eqs. (2.1) and (2.2) lead to $a_{eff} = a_c = b$, as it must be. Finally, in terms of the initial dimensional variables, a_c and b , the effective trapping radius is given by

FIG. 1. Spiky absorbers: (a) the absorber formed by 4 absorbing spikes of length h protruding from the absorbing core of radius a_c and (b) no-core absorbers formed by 1, 2, and 4 absorbing spikes of length h . Dashed circles are effective circular absorbers.

$$a_{\text{eff}} = \frac{1}{b} \left(\frac{a_c^n + b^n}{2} \right)^{2/n}. \quad (2.4)$$

The effective trapping circles are shown in Fig. 1 by dashed lines.

III. NUMERICAL TEST

To test the accuracy of the replacement of our complex-shaped absorber by an effective circular one, we consider trapping of a particle diffusing inside a circular domain constrained by a reflecting boundary, with our absorber located in the center of the domain. The mean particle lifetime obtained from Brownian dynamics simulations is compared with the mean lifetime predicted by the theory for the case of a circular absorber of radius a . The latter mean lifetime, denoted by $\tau(r \rightarrow a | R_{rb})$, is given by (see the derivation in the Appendix)

$$\tau(r \rightarrow a | R_{rb}) = \frac{1}{4D} \left[2R_{rb}^2 \ln \left(\frac{r}{a} \right) - (r^2 - a^2) \right], \quad (3.1)$$

where R_{rb} is the radius of the outer reflecting boundary (rb) circle, r is the initial distance of the particle from the origin, $a \leq r \leq R_{rb}$, and D is the particle diffusivity. When it is possible to replace our spiky absorber by an effective circular absorber, the mean lifetimes obtained from the simulations and given by Eq. (3.1) with $a = a_{\text{eff}} = bF(n, \varepsilon)$ must be equal. With this in mind, we substitute the former mean lifetime into the left-hand side of Eq. (3.1) and solve the resulting equation with

TABLE I. The n -dependence of the ratio $a_{\text{eff}}/b = F(n, 0) = 1/2^{2/n}$ for no-core absorbers.

n	1	2	4	8	16
$F(n, 0)$	0.25	0.5	0.7071	0.8408	0.9170

respect to the absorber radius, which we denote $a_{\text{eff}}^{\text{sim}}$. Then we compare $a_{\text{eff}}^{\text{sim}}$ with a_{eff} given by Eq. (2.1).

In simulations, the particle starting point was uniformly distributed over the circle of radius b . For this initial condition, $r = b$, Eq. (3.1) reduces to

$$\frac{4D}{b^2} \tau(b \rightarrow a | R_{rb}) = - \left\{ 2 \left(\frac{R_{rb}}{b} \right)^2 \ln \left(\frac{a}{b} \right) + \left[1 - \left(\frac{a}{b} \right)^2 \right] \right\}. \quad (3.2)$$

We find the ratio $a_{\text{eff}}^{\text{sim}}/b$ by solving this equation with $\tau(b \rightarrow a | R_{rb})$ replaced by the mean particle lifetime obtained from the simulations. This ratio is then compared with the function $F(n, \varepsilon)$ given by Eq. (2.2). The comparison is made in two steps: first, for no-core absorbers, the focus is on the n -dependence predicted by Eq. (2.3), and then we study the ε -dependences at fixed values of n predicted by Eq. (2.2).

A. No-core absorber

The n -dependence of the ratio a_{eff}/b for no-core absorbers, $\varepsilon = 0$, is described by the function $F(n, 0)$ given in Eq. (2.3). This ratio monotonically increases with n from 0.25 at $n = 1$ to unity as $n \rightarrow \infty$. The n -dependence of the ratio is illustrated in Table I. Note that the no-core absorbers with $n = 1$ and 2 are formally identical because both are absorbing intervals of the lengths h and $2h$, respectively [see Fig. 1(b)]. This is the reason why the radius of the effective absorbing circle for $n = 2$ is twice longer than that for $n = 1$. The relation between the length of a linear absorber and the radius of the equivalent absorbing circle was obtained by Szabo *et al.*,¹⁰ as well as in potential theory.¹¹ The fundamental difference between the two absorbing intervals lies in their locations with respect to the origin: symmetric for $n = 2$ and asymmetric for $n = 1$ [see Fig. 1(b)].

Our simulation results for the no-core absorbers are presented in Table II, which gives the ratios $a_{\text{eff}}/a_{\text{eff}}^{\text{sim}}$ for $n = 1, 2, 4, 8$, and 16, at different radii of the reflecting boundary circle, $R_{rb}/b = 1, 2, 4, 8$, and 10. One can see that for $n = 8$ and 16, the ratio is practically unity for all R_{rb} , starting with $R_{rb} = b$. For

TABLE II. The ratios of $a_{\text{eff}}/a_{\text{eff}}^{\text{sim}}$ for no-core absorbers formed by $n = 1, 2, 4, 8$, and 16, spikes at different radii of the reflecting boundary circle $R_{rb}/b = 1, 2, 4, 8$, and 10.

		R_{rb}/b				
		1	2	4	8	10
n	1	1.152	1.082	1.066	1.047	1.008
	2	1.044	1.008	1.006	1.012	1.018
	4	1.024	1.009	1.012	0.999	1.013
	8	1.009	1.007	1.000	0.994	1.009
	16	1.014	1.015	1.008	1.012	1.005

FIG. 2. Core radius dependence of the radius a_{eff} of the effective circular trap for spiky absorbers with $n = 1, 2, 4$, and 8 spikes (solid lines from bottom to top). Symbols are the values of the $a_{\text{eff}}^{\text{sim}}/b$ ratio obtained from simulations with $R_{rb} = 10$.

$n = 2$ and 4 , the ratio is larger than unity by 4.5% and 2.5%, respectively, at $R_{rb} = b$ and is practically unity for $R_{rb} \geq 2b$. For $n = 1$, the ratio approaches unity, as R_{rb} increases, slower than that for other n because of the asymmetric location of the absorber with respect to the origin [see Fig. 1(b)].

B. Core radius dependence

The effective radius dependence on the core radius is determined by the ε -dependences of the function $F(n, \varepsilon) = a_{\text{eff}}/b$. As ε increases from zero to unity, $F(n, \varepsilon)$, Eq. (2.2), increases from $F(n, 0) = 1/2^{2/n}$ to $F(n, 1) = 1$. The ε -dependences of this function are shown in Fig. 2 by solid lines for $n = 1, 2, 4$, and 8 . Symbols in Fig. 2 are the values of the ratio $a_{\text{eff}}^{\text{sim}}/b$ obtained from simulations with the same values of n and $\varepsilon = 0, 0.25, 0.5$, and 0.75 at $R_{rb} = 10$. One can see excellent agreement between the theoretical predictions and the simulation results.

IV. DERIVATION

The procedure of replacement of a spiky absorber by an effective circular absorber is an example of the approach referred to in the literature as boundary smoothing. Recently, Skvortsov and Walker¹² considered smoothing of an absorbing comb-like boundary shown in Fig. 3, which consists of

FIG. 3. Absorbing comb-like boundary formed by periodic absorbing spikes of height H protruding from the absorbing base. The spikes are separated by the comb period W . The dashed line is the effective flat absorbing boundary located at distance Δ below the spike tops.

infinitely thin absorbing spikes of height H protruding from an absorbing base. The spikes are separated by the comb period W . These authors demonstrated that trapping by such a boundary is equivalent to trapping by a flat absorbing boundary (shown in Fig. 3 as a dashed straight line), which is located at distance Δ below the spike tops. The relation between Δ , H , and W is given by

$$\Delta = \frac{W}{\pi} \ln \left[\frac{2}{1 + \exp(-2\pi H/W)} \right]. \quad (4.1)$$

To derive the expression for the radius a_{eff} of the effective circular absorber, Eq. (2.1) with the function $F(n, \varepsilon)$ in Eq. (2.2), we convert our spiky absorber into a comb-like absorber shown in Fig. 3. This can be done by changing the initial polar coordinates r and φ to Cartesian coordinates x and y ,

$$x(r, \varphi) = b\varphi, \quad y(r, \varphi) = b \ln(r/b), \quad (4.2)$$

where x corresponds to the horizontal coordinate along the comb, and y is the distance from the bottom of the comb. Then the period W and the spike height H of the comb-like boundary are related to the absorber parameters b , n , and ε by the relations

$$W = 2\pi b/n, \quad H = -b \ln \varepsilon. \quad (4.3)$$

An important property of the coordinate transformation in Eq. (4.2) is that it conserves the total flux over the period. Therefore, the total fluxes over the period in Cartesian and polar coordinates are equal.

Substituting W and H given in Eq. (4.3) into Eq. (4.1), we obtain

$$\Delta = \frac{2b}{n} \ln \left(\frac{2}{1 + \varepsilon^n} \right). \quad (4.4)$$

As follows from Eq. (4.2), the relation between Δ and a_{eff} is given by

$$\Delta = b \ln(a_{\text{eff}}/b). \quad (4.5)$$

Finally, combining Eqs. (4.4) and (4.5), we arrive at the expression for the radius of the effective circular absorber in Eq. (2.1) with the function $F(n, \varepsilon)$ in Eq. (2.2).

V. CONCLUDING REMARKS

In summary, to describe trapping of diffusing particles by a spiky absorber (see Fig. 1), we replace this absorber by an effective circular absorber, for which the trapping problem can be solved with relative ease. Our main result is the expression for the radius a_{eff} of the effective absorber, Eqs. (2.1) and (2.2), which, from the trapping point of view, is equivalent to the initial spiky absorber. Mean particle lifetimes obtained from Brownian dynamics simulations with various spiky absorbers are in excellent agreement with the mean lifetimes predicted by the theory using a_{eff} .

Our derivation of a_{eff} exploits a recent result by Skvortsov and Walker¹² who showed that trapping by an absorbing comb-like boundary can be described as trapping by a correctly located flat boundary (see Fig. 3). In this paper, we extended their result to the circular geometry using the transformation in Eq. (4.2). While we compare the mean particle lifetimes obtained from simulations and predicted by the theory, in Ref. 12 the authors demonstrated excellent agreement not only

for the mean value (which is the first moment) but also for the distribution of this random variable. Since our derivation is an extension of the result in Ref. 12, we believe that the boundary smoothing approach applied in the circular geometry also leads to an accurate estimate of the distribution and hence all moments of the particle lifetime.

Although our analysis above focuses on spiky absorbers in two dimensions, the boundary smoothing approach can also be applied to other complex-shaped absorbers in two and three dimensions. The point is that at the large distances from any absorber the tangential component of the flux vanishes and only its radial component survives. This eventually enables the replacement of a complex-shaped absorber by an effective circular or spherical absorber in two and three dimensions, respectively. The difficulty is in finding an expression for the radius of the effective absorber. Here we obtained the expression for a_{eff} by transforming the result for the location of the equivalent flat boundary from Ref. 12, which was derived using the conformal invariance of the Laplace equation. Since conformal invariance is the property of the Laplace equation (with proper boundary conditions) in two dimensions, this approach cannot be used to find the effective radius of a complex-shaped absorber in three dimensions.

ACKNOWLEDGMENTS

A.S. thanks Ian MacGillivray for useful discussions and comments. A.M.B. and L.D. are grateful to Sergey Bezrukov, and A.M.B. is grateful to Irina Gopich and Attila Szabo for helpful discussions. This study was partially supported by the Intramural Research Program of the National Institutes of Health, the Center for Information Technology.

APPENDIX: DERIVATION OF EQ. (3.1)

Consider a particle diffusing in an annulus bounded by an absorbing inner circle of radius a and a reflecting outer

circle of radius R_{rb} . The mean particle lifetime, considered as a function of its initial distance r from the circle center, $a \leq r \leq R_{rb}$, is the mean first-passage time of the particle from r to the absorbing inner circle. This time, denoted by $\tau(r \rightarrow a | R_{rb})$, satisfies¹³

$$\frac{D}{r} \frac{d}{dr} \left(r \frac{d\tau}{dr} \right) = -1, \quad (\text{A1})$$

subject to the boundary conditions

$$\tau|_{r=a} = \left. \frac{d\tau}{dr} \right|_{r=R_{rb}} = 0. \quad (\text{A2})$$

Integrating Eq. (A1) and using the boundary condition at $r = R_{rb}$, we obtain

$$\frac{d\tau}{dr} = \frac{1}{2D} \left(\frac{R_{rb}^2}{r} - r \right). \quad (\text{A3})$$

Integrating this with the absorbing boundary condition at $r = a$, we arrive at the expression for the mean particle lifetime, $\tau(r \rightarrow a | R_{rb})$, in Eq. (3.1).

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