Mapping of diffusion in a channel with abrupt change of diameter

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Mapping of the diffusion equation in a channel of varying cross section onto the longitudinal coordinate is already a well studied procedure for a slowly changing radius. We examine here the mapping of diffusion in a channel with abrupt change of diameter. In two dimensions, our considerations are based on solution of the exactly solvable geometry with abruptly doubled width at $x=0$. We verify the surmise of Berezhkovskii *et al.* [J. Chem. Phys. **131**, 224110 (2009)] that one-dimensional diffusion behaves as free in such channels everywhere except at the point of change, which looks like a local trap for the particles. Applying the method of "sewing" of solutions, we show that this picture is valid also for three-dimensional symmetric channels.

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I. INTRODUCTION

Increasing interest in nanomaterials and biological systems in the last decade has motivated numerous studies of transport in quasi-one-dimensional (quasi-1D) structures, such as pores, channels, along fibers, etc. The most effective description of such systems is purely one-dimensional, not dealing with the less interesting motion of particles across the channel, but representing correctly all its important effects on transport in the longitudinal direction.

Our system of interest is diffusion in a channel with varying cross section. Mapping of the original d dimensional ($d=2,3$) diffusion equation

$$\frac{\partial \rho(x,\mathbf{y},t)}{\partial t} = \left[D_0 \frac{\partial^2}{\partial x^2} + D_t \sum_{j=1}^{d-1} \frac{\partial^2}{\partial y_j^2} \right] \rho(x,\mathbf{y},t), \tag{1}$$

in the channel with reflecting walls onto the longitudinal coordinate x is already well understood when the cross section $A(x)$ is a smooth and slowly varying function. The simplest 1D equation which reasonably replaces Eq. (1) is the Fick-Jacobs (FJ) equation [1].

$$\frac{\partial p(x,t)}{\partial t} = D_0 \frac{\partial}{\partial x} A(x) \frac{\partial}{\partial x} \frac{p(x,t)}{A(x)}, \tag{2}$$

governing the 1D density $p(x,t)$

$$p(x,t) = \int_{A(x)} \rho(x,\mathbf{y},t) d\mathbf{y}, \tag{3}$$

the integral of the d-dimensional density $\rho(x,\mathbf{y},t)$ over the transverse coordinates $\mathbf{y}=(y_1,\ldots,y_{d-1})$; $D_0=D_t$ is the diffusion constant, and $A(x)$ denotes both the cross section and its area.

The FJ equation takes only the longitudinal mass conservation into account. One arrives at this equation if the transverse relaxation is infinitely fast, which is equivalent to a channel of negligible width in comparison with the typical longitudinal length scale. In practice, FJ equation has to be corrected; the analysis of Zwanzig [2] and Reguera and Rubí [3] showed that the correction should has the form

$$\frac{\partial p(x,t)}{\partial t} = \frac{\partial}{\partial x} A(x) D(x) \frac{\partial}{\partial x} \frac{p(x,t)}{A(x)}, \tag{4}$$

where $D(x)$ is an effective diffusion coefficient, a function estimated by the formula

$$D(x) = D_0 / \sqrt{1 + R'^2(x)}, \tag{5}$$

for three-dimensional (3D) symmetric channels of radius $R(x)$; here, $A(x)=\pi R^2(x)$.

An exact mapping procedure [4–7], based on introducing anisotropy of the diffusion constant in the diffusion Eq. (1), taking the transverse constant $D_t=D_0/\epsilon$ much larger than D_0, enables us to find systematically the corrections to the FJ Eq. (2) up to an arbitrary order in the small parameter ϵ. Then in the limit of stationary flow (i.e., at nearly a constant net flux through the channel), the ϵ expansion of $D(x)$ can be expressed explicitly,

$$\frac{D(x)}{D_0} = 1 - \frac{\epsilon}{2} R'^2 + \frac{\epsilon^2}{48} R' (18R'^3 + 3RR'R'' - R^2 R^{(3)}) - \cdots \tag{6}$$

for 3D symmetric channels [6]. The formula (5) correctly sums the terms depending only on $R'(x)$ at $\epsilon=1$. Aside from them, the exact $D(x)$ also depends on the higher derivatives of $R(x)$ of any order, which are neglected in Eq. (5). Numerical tests [8] exhibited its validity restricted to not very steep changes of $R(x)$: $|R'(x)|<1$.

Many tasks in practice, e.g., particles diffusing between cavities, or escaping from a cavity through a long narrow tunnel, require solving the situation when $R(x)$ or $A(x)$ changes abruptly. $R'(x)$ becomes infinite at the point of change and use of the formula (5) is dubious. Some problems of this kind were solved by Berezhkovskii *et al.* [9–12]. We revisit the simplest of these, a channel consisting of two straight cylinders of different radius; $R(x)=a$ for $x>0$ and $R(x)=b$ for $x<0$. At $x=0$, the parts are connected by a flat hard wall (reflecting) annular fitting.

Berezhkovskii *et al.* approximated the connection as a trap for the transiting particles [11]. They are partially absorbed at $x=0$ with specific trapping rates from left and right, but diffuse freely elsewhere in both parts of the channel. Using this 1D description in calculation of the mean first passage time, the authors arrived at results in excellent agreement with the numerical solution of the full 3D problem.

The aim of our paper is to validate this approximation within the context of our exact mapping procedure. At first sight, the concept of a local trap at $x=0$ seems to be a rough approximation. The abrupt change of radius of the channel influences the stationary 3D density in a wide vicinity of $x=0$ and so one could expect that diffusion in this transition region cannot be considered as free even in the 1D picture. Also the coefficient $D(x)$ depending on the derivatives of $R(x)$ implies a nonlocal relation between the radius $R(x)$ and the 1D diffusivity.

On the other hand, the recurrence mapping procedure, generating the exact expansion of $D(x)$ Eq. (6), requires the function $R(x)$ to be analytic, and its direct adoption for $R(x)$ approaching the step function becomes dubious.

In our analysis, we utilize calculation of $D(x)$ from the stationary density $p(x)$ Eq. (3), if it is known explicitly for some exactly solvable geometry [13]. Then

$$\frac{1}{D(x)} = -\frac{1}{J}A(x)\frac{d}{dx}\frac{p(x)}{A(x)}, \tag{7}$$

J denotes the net flux corresponding to the stationary density $p(x)$. According to Ref. [13], the resultant $D(x)$ represents the sum of the expansion of $D(x)$ in ϵ, and so this method is equivalent to the exact mapping in the limit of the stationary flow.

In Sec. II, we show that the two-dimensional (2D) version of the stepwise channel is exactly solvable. For a specific ratio b/a, we derive explicit 2D density $\rho(x,y)$ using conformal transformation in the complex plane. Despite complicated $\rho(x,y)$ near $x=0$, we find that the 1D density $p(x)$ has a simple form

$$p(x) = -J[x + C_t\Theta(x) + C_0] + A(x)\rho_0, \tag{8}$$

$\Theta(x)$ denotes the Heaviside unit step function, C_t, C_0 are constants depending on geometry (a and b) and ρ_0 is an equilibrium 2D density.

Next, we give arguments that $p(x)$ preserves the form Eq. (8) for any a and b. The formalism in the complex plane can be used only for 2D channels. In Sec. III, we derive a complementary formalism based on "sewing" of solutions in both parts of the channel, which is also usable in 3D. We demonstrate that the stationary density $p(x)$ in the 3D channels is of the form Eq. (8), too.

The 1D density $p(x)$ grows linearly everywhere, even in the vicinity of $x=0$, but it exhibits a jump at $x=0$. If applied in Eq. (7), $1/D(x)=1$ everywhere except at $x=0$, where we observe a singularity. This picture corresponds exactly to the concept of a local trap at $x=0$ and free 1D diffusion elsewhere, as supposed by Berezhkovskii.

II. CONFORMAL TRANSFORMATION

We will now study the stationary diffusion in a 2D channel with a step at $x=0$, bounded by the x axis and a function $A(x)$

$$A(x) = b + (a-b)\Theta(x); \tag{9}$$

the 2D density $\rho(x,y)$ satisfies reflecting (Neumann) boundary conditions (BC) on the walls, including the transverse connection between the left and right parts at $x=0$.

First we recall briefly the formalism of calculating $D(x)$ in the complex plane (explained in Ref. [13], Appendix B). We work with the coordinates $z=x+iy$, $\bar{z}=x-iy$. Any analytic complex function $f(z)$ is a solution of the Laplace equation $\Delta f(z)=\partial_z\partial_{\bar{z}}f(z)=0$, which is also valid for its components

$$Jf(z) = \phi(x,y) + i\rho(x,y). \tag{10}$$

The conditions

$$\text{Re } f(x) = 0, \quad \text{Re } f[x + iA(x)] = 1, \tag{11}$$

together with the Cauchy-Riemann relations for ϕ and ρ fix the Neumann BC for Im $f(z)$ at the boundaries $y=0,A(x)$ and so $\rho(x,y)$ in Eq. (10) can be interpreted as the 2D stationary density in the channel, carrying the total flux J.

The primitive function $g(z)=\int f(z)dz$ directly determines the 1D density $p(x)=J\,\text{Re}\{g(x)-g[x+iA(x)]\}$, hence the formula (7) becomes

$$\frac{1}{D(x)} = A(x)\frac{d}{dx}\left(\frac{1}{A(x)}\text{Re}\{g[x+iA(x)] - g(x)\}\right). \tag{12}$$

As an example, we consider the function

$$f(z) = -\frac{i}{\phi_0}\ln z = -\frac{i}{\phi_0}\ln(x+iy). \tag{13}$$

Its imaginary part Im $f(z)=-(1/2\phi_0)\ln(x^2+y^2)$ represents the stationary density $\rho(x,y)$ from a pointlike source placed at the origin, supplying the unit flux J to the corner bounded by the positive part of the x axis, where Re $f(x>0)=0$, and the line $y=A(x)=x\tan\phi_0$, where Re $f(x+ix\tan\phi_0)=1$; this is a wedge of angle ϕ_0. Satisfying the Neumann BC is apparent from the symmetry. The corresponding primitive function $g(z)=-(i/\phi_0)(z\ln z-z)$ then determines $p(x)$ and according to Eq. (12), we obtain $D(x)=\phi_0/\tan\phi_0=[\arctan A'(x)]/A'(x)$ (see Ref. [13].).

Any conformal transformation $z=\chi(w)$ (and its conjugate) preserves the original BC of the transformed function $h(w)=f[\chi(w)]$ on the transformed boundaries in the new complex variable $w=u+iv$. The Laplacian is transformed as $\partial_z\partial_{\bar{z}}=|\chi'(w)|^{-2}\partial_w\partial_{\bar{w}}$ and thus also $h(w)$ satisfies the Laplace equation $\partial_w\partial_{\bar{w}}h(w)=0$. So we can apply the same formalism on $h(w)$ as before on $f(z)$ to calculate the stationary densities $\rho(u,v)$, $p(u)$ and finally $D(u)$ in the new geometry.

In the present case, we choose

$$w = \text{arccosh}\left(\frac{2z-k-1}{k-1}\right) - \frac{1}{\sqrt{k}}\text{arccosh}\left(\frac{(k+1)z-2k}{(k-1)z}\right), \tag{14}$$

transforming the upper half plane (x,y) onto the steplike channel in the variables u,v [see Figs. 1(a) and 1(b)]. The positive part of the x axis transforms to the lower boundary, broken at $w=0$ and $i\pi(1-1/\sqrt{k})$, corresponding to $z=k$ and 1, when the argument of the first arccosh becomes ±1. The negative part of the x axis transforms to the flat upper boundary at $v=\pi$ and the source of particles at $z=0$ has its image

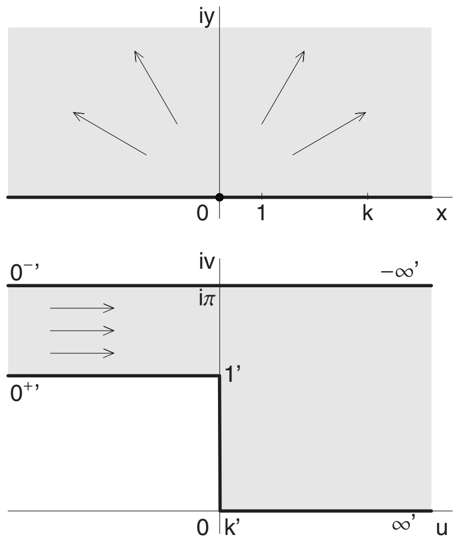

FIG. 1. Conformal transformation [Eq. (14)] transforms the upper half plane (the upper figure) onto the stepwise channel (the lower figure).

at $-\infty$ inside the channel. The parameter k regulates the ratio of widths $b/a=\sqrt{k}$ of the wide and narrow parts of the channel. Note that (inverse) mapping the transverse source at $-\infty$ to the single point $z=0$ supplies uniqueness to the 1D projection.

The half plane $y>0$ can be taken as a corner of angle $\phi_0=\pi$ studied above. The function $f(z)$, which satisfies the required BCs for the half plane, is given by Eq. (13) for $\phi_0=\pi$. So the corresponding function $h(w)$, describing the stationary flow in the step-wise channel is

$$h(w) = -\frac{i}{\pi}\ln[\chi(w)], \tag{15}$$

where $\chi(w)$ is the inverted relation (14). For a few values of k, we can express the function $\chi(w)$ and so $h(w)$ explicitly (see Appendix).

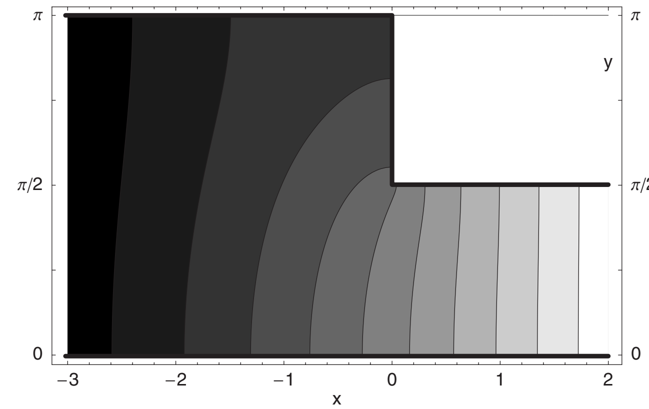

FIG. 2. Contour plot of the 2D density $\rho(x,y)$ in a channel of widths $a=\pi/2$ and $b=\pi$ for $x>0$ and $x<0$, respectively.

For our demonstration purposes, we consider only $k=4$, corresponding to the widths $a=\pi/2$ and $b=\pi$. Skipping the tedious algebra, we state the final formula for the rotated and shifted (u,v) plane, $w=u+iv=i\pi-x-iy=i\pi-s$, turning the channel to the desired position with the flat boundary identical with the x axis,

$$h(s) = \frac{3i}{\pi}\ln\left[1-e^{-2i\pi/3}\left(\frac{1+ie^{s}}{1-ie^{s}}\right)^{2/3}\right] + \frac{i}{\pi}\ln[2(1-i\sinh s)] + 1 + i\rho_0/J = (\phi(x,y)+i\rho(x,y))/J, \tag{16}$$

consistent with Eq. (10). We added an imaginary constant $i\rho_0/J$, which does not influence either the Neumann BC, or the values $\mathrm{Re}[h(s)]=0,1$ at the lower and upper boundaries. ρ_0 represents an equilibrium density, or a constant fixing $\rho(x_{l,r},y)=0$ at a distant absorbing left or right end of a real channel ($|x_{l,r}|\gg a,b$). The density $\rho(x,y)$ according to Eq. (16) is depicted in the contour graph in Fig. 2.

Now, from the primitive function $g(s)=\int h(s)ds$,

$$g(s) = \frac{is}{J}\rho_0 + s + \frac{3i}{\pi}\Big(\frac{1}{3}\mathrm{Li}_2[-ie^{-s}] - \frac{1}{3}\mathrm{Li}_2[ie^{s}] + \mathrm{Li}_2[e^{-i\pi/3}(1-q)] - \mathrm{Li}_2[e^{-i\pi/3}(1+q)] + \mathrm{Li}_2[e^{i\pi/3}(1-q)] - \mathrm{Li}_2[e^{i\pi/3}(1+q)]$$
$$+ \mathrm{Li}_2[(1-q)/2] - \mathrm{Li}_2[(1+q)/2] - \mathrm{Li}_2\left[\frac{1-q}{1+e^{-i\pi/3}}\right] + \mathrm{Li}_2\left[\frac{1+q}{1+e^{-i\pi/3}}\right] - \mathrm{Li}_2\left[\frac{1-q}{1+e^{i\pi/3}}\right] + \mathrm{Li}_2\left[\frac{1+q}{1+e^{i\pi/3}}\right] - \ln(1+q)$$
$$\times\left[\ln\frac{3i}{2}e^{-s} + \frac{1}{2}\ln(1+q)\right] + \ln(1-q)\left[\ln\frac{3}{2i}e^{s} + \frac{1}{2}\ln(1-q)\right]\Big), \tag{17}$$

where $q=e^{-i\pi/3}[(1+ie^{s})/(1-ie^{s})]^{1/3}$ and $\mathrm{Li}_2(z)=-\int_0^z dx\,\ln(1-x)/x$ denotes the polylogarithm function, we find the 1D density

$$p(x) = J\,\mathrm{Re}[g(x)-g(x+iA(x))] = -J(x+C_t\Theta(x)+C_0)+A(x)\rho_0. \tag{18}$$

The constants C_t, C_0 are given by

$$C_t = \mathrm{Re}[g(0^+ + i\pi/2) - g(0^- + i\pi)] = 1.21640$$

$$C_0 = \mathrm{Re}[g(0^- + i\pi) - g(0)] = -1.64792. \tag{19}$$

According to Eq. (12), $D(x)=1$ for any $x\neq 0$.

We can avoid the tedious calculation of $h(s)$ and $g(s)$. For $x\neq 0$, the formula (12) reduces to

$$\frac{1}{D(x)} = \frac{d}{dx}\mathrm{Re}[g(x+iA) - g(x)], \quad (20)$$

as $A(x)=A$ is constant (a or b). Next,

$$\frac{1}{D(x)} = \mathrm{Re}[\partial_s g(s)|_{s=x+iA} - \partial_s g(s)|_{s=x}] = \mathrm{Re}[h(x+iA) - h(x)]$$
$$= \phi(x,A) - \phi(x,0) = 1. \quad (21)$$

Consequently, we need not express $h(s)$ explicitly, and Eq. (21) is valid for any k, i.e., for any ratio b/a, and in fact for any flat portion of a 2D channel.

It is instructive to compare this result with the Fick-Jacobs approximation, which supposes infinitely fast relaxation in the transverse direction. Then the 2D density $\rho(x,y)=\rho(x)$ does not depend on y, $\rho(0^+)=\rho(0^-)$ and thus the stationary $p(x)=A(x)\rho(x)=-Jx+A(x)\rho_0$ to preserve mass conservation. Taking the true relaxation into account, we gain an extra jump of $p(x)$ by $-JC_t$ at $x=0$, due to the particles moving slowly along the transverse wall in the y direction, i.e., stationary if watched only in the 1D picture. The point $x=0$ looks then like a trap. The trap is local, as $D(x)=1$ everywhere else and so the 1D diffusion there is really free.

Finally, combining Eqs. (7) and (18), we arrive at the relation

$$\frac{1}{D(x)} = A(x)\frac{d}{dx}\left[\frac{x + C_t\Theta(x) + C_0}{A(x)}\right]$$
$$= 1 + [bC_t + (b-a)C_0]\frac{\delta(x)}{A(x)}. \quad (22)$$

To avoid ambiguity in fixing $\delta(x)/A(x)$ at $x=0$, we recommend using the first "raw" formula (22) in practical calculations [14].

III. SEWING OF SOLUTIONS

Due to using the complex plane formalism, our consideration in the previous Section is restricted only to 2D channels. We present now a complementary calculation, enabling us to extend our technique to 3D channels.

The method is based on the fact that the steady state diffusion problem can be decomposed into two separate diffusion problems in half planes to the left and right of the abrupt width change with impermeable boundaries at $x=0$ and suitably chosen sink/source terms. For the channel, defined by the function (9) (Fig. 3), we suppose that the particles diffusing from e.g., left side of width $b \geq a$ are absorbed just before $x=0$ along the cross section $0<y<a$ with some distribution $\tau(y)$ and immediately after $x=0$ injected to the opposite part. The transverse boundary $a \leq y < b$ at $x=0$ is reflecting. The same distribution $\tau(y)$ of absorption from the left and injection to the right mimics the steady state flux density through the step of the channel. Our task then is to find $\tau(y)$ such that the 2D stationary density will be continuous at $x=0$, $\rho(0^-,y)=\rho(0^+,y)$ for $0<y<a$. The corresponding integral equation also fixes the constant C_t.

Consider first the 2D case. The procedure exploits our knowledge of the stationary density around a pointlike

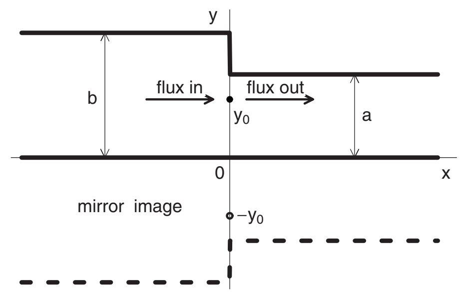

FIG. 3. Shape of the 2D channel.

source in a flat channel of width a placed at a point $(0,y_0)$, $y_0<a$. In the 2D channel, we have the expression

$$\rho(x,y|y_0) = -\frac{J}{2\pi}\ln\left[\left(\cosh\frac{\pi x}{a} - \cos\frac{\pi}{a}(y-y_0)\right)\right.$$
$$\left.\times\left(\cosh\frac{\pi x}{a} - \cos\frac{\pi}{a}(y+y_0)\right)\right] + C_L, \quad (23)$$

on solving the Laplace equation with Neumann BC at the walls $y=0$ and a (see Appendix). For $|x| \gg a$, the contribution of cosine in Eq. (23) becomes negligible, the 2D density depends only on x, so the constant C_L can fix ρ to zero at distant absorbing ends of the channel, $x=\pm L$. The density [Eq. (23)] corresponds to the total flux $\pm J$ on the right and the left side of the source.

We can consider now only the right part of the channel, $0<x<L$, with the particles injected along the (reflecting) wall at $x=0$, distributed according to the function $\tau(y_0)=\tau(-y_0)$. Then the 2D density is

$$\rho(x,y) = C_a - \int_{-a}^{a}\tau(y_0)\ln\left[\cosh\frac{\pi x}{a} - \cos\frac{\pi}{a}(y-y_0)\right]dy_0 \quad (24)$$

(using also integration across the mirror image of the channel, see Fig. 3). The same calculation can be done for the left side of the channel, but now, we suppose that its width is $b \geq a$,

$$\rho(x,y) = C_b + \int_{-a}^{a}\tau(y_0)\ln\left[\cosh\frac{\pi x}{b} - \cos\frac{\pi}{b}(y-y_0)\right]dy_0. \quad (25)$$

Instead of injecting, the particles are drained at $x=0$ with the same distribution, hence $\tau(y_0)$ was replaced by $-\tau(y_0)$. No particles are drained for $a<|y_0|<b$, the Neumann BC there is maintained by construction of the 2D density.

Finally, we provide the "sewing," $\rho(0^+,y)=\rho(0^-,y)$ for $|y|<a$. Combining Eqs. (24) and (25), we get an integral equation

$$\int_{-a}^{a}\tau(y_0)\ln\left[\left(1 - \cos\frac{\pi(y-y_0)}{a}\right)\times\left(1 - \cos\frac{\pi(y-y_0)}{b}\right)\right]dy_0$$
$$= C_a - C_b, \quad (26)$$

fixing the function $\tau(y_0)$ and the difference $C_a - C_b$.

The function $\tau(y_0)$ is seen to be proportional to the longitudinal current density $j_x(x,y_0)=-\partial_x\rho(x,y_0)$ at $x=0^+$. From Eq. (24),

$$j_x(0^+,y) = \int_{-a}^{a} \frac{(\pi/a)\sinh(\pi x/a)\tau(y_0)dy_0}{\cosh(\pi x/a)-\cos[\pi(y-y_0)/a]}\bigg|_{x\to 0^+} = \int_{-a}^{a} 2\pi\delta(y-y_0)\tau(y_0)dy_0 = 2\pi\tau(y) \quad (27)$$

and the total flux is

$$J = \int_0^a j_x(0^+,y)dy = 2\pi\int_0^a \tau(y)dy. \quad (28)$$

The function $\tau(y_0)$ and thus also C_a-C_b can be scaled by J. If $b=a$, the solution of Eq. (26) is $\tau(y_0)=J/(2\pi a)$ and the corresponding $C_a-C_b=-(J/\pi)\ln 4$. Then it is convenient to define $C_a-C_b=-J[C+(1/\pi)\ln 4]$, where C depends only on a and b and equals zero for the flat channel.

Integration of Eqs. (24) or (25) over the cross section gives the 1D density $p(x)$,

$$p(x) = AC_A - \text{sgn}(x)\int_{-a}^{a}\tau(y_0)dy_0 \times \int_0^A \ln\left[\cosh\frac{\pi x}{A} - \cos\frac{\pi(y-y_0)}{A}\right]dy = AC_A - J\left(x - \text{sgn}(x)\frac{A}{\pi}\ln 2\right), \quad (29)$$

$A=a$ for $x>0$ and $A=b$ for $x<0$. Comparing this result with Eq. (18), we find

$$C_a = \rho_0 - J[(C_t+C_0)/a + (1/\pi)\ln 2],$$

$$C_b = \rho_0 - J[C_0/b - (1/\pi)\ln 2], \quad (30)$$

hence the relation between C_t, C_0, and C reads

$$C_a - C_b + \frac{J}{\pi}\ln 4 = -JC = -J\left(\frac{C_t+C_0}{a} - \frac{C_0}{b}\right). \quad (31)$$

There is ambiguity in setting C_t, C_0. If δ is added to C_t and $b\delta/(a-b)$ to C_0, the relation (31) holds and ρ_0 in Eq. (18) increases by $J\delta/(a-b)$. We can set $C_0=0$ and then $C_t=aC$. The constant ρ_0 is then fixed to satisfy the Dirichlet BC at the absorbing end of the channel.

The calculation presented can be verified in the exactly solvable case $a=\pi/2$, $b=\pi$. The function $\tau(y)$ related to the density $\rho(x,y)$ from Eq. (16),

$$\tau(y) = \frac{\sqrt{3}J}{4\pi^2}\left(\sqrt[3]{\frac{\cos y}{1+\sin y}} + \sqrt[3]{\frac{1+\sin y}{\cos y}}\right), \quad (32)$$

solves the integral Eq. (26), giving the constant $C=(3/2\pi)\ln(27/16)=0.24983$. One can check that C_t, C_0 from Eqs. (19) satisfy the relation (31) with this value of C. Details of this calculation are given in the Appendix.

Extension of this method to 3D symmetric channels is straightforward. We consider a channel of radius

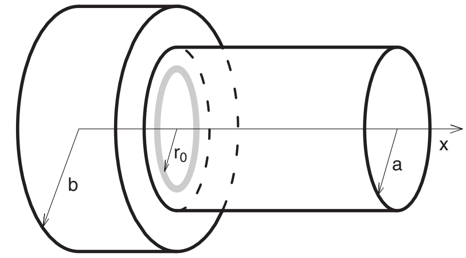

FIG. 4. Shape of the 3D channel.

$$R(x) = b + (a-b)\Theta(x), \quad (33)$$

$b\geq a$ (Fig. 4). The 3D density $\rho(x,r)$ (in cylindrical coordinates, not depending on the angle ϕ) has the form

$$\rho(x,r) = C_R + \text{sgn}(x)\int_0^a G_R(x,r|r_0)\tau(r_0)dr_0, \quad (34)$$

R denotes a, b for $x>0$ and $x<0$, respectively. The function $G_R(x,r|r_0)$ represents the stationary density generated by the source shaped as an infinitesimally thin ring of radius r_0 placed symmetrically in the infinite cylinder of radius R at $x=0$. The function $\tau(r_0)$, determining the distribution of the current density $j_x(x,r)$ across the radius at $x=0$, is taken with opposite signs for the left and right parts to provide the local mass conservation. Finally, sewing of the solutions in both parts, $\rho(0^+,r)=\rho(0^-,r)$, yields the equation

$$\int_0^a \tau(r_0)[G_a(0^+,r|r_0) + G_b(0^-,r|r_0)]dr_0 = C_b - C_a, \quad (35)$$

fixing the function $\tau(r_0)$ and C_b-C_a.

In our next analysis, we use $G_R(x,r|r_0)$ written as

$$G_R(x,r|r_0) = \frac{1}{\pi R^2}\left[-|x| + \sum_{n=1}^{\infty} e^{-k_n|x|}\frac{J_0(k_nr_0)J_0(k_nr)}{k_nJ_0^2(k_nR)}\right] \quad (36)$$

(derived in the Appendix), $J_\nu(z)$ denotes the Bessel functions and k_n runs over the roots of $J_1(k_nR)=0$. Using this formula in Eq. (34), we calculate the total flux,

$$J = -\int_0^a 2\pi r\partial_x\rho(x,r)dr|_{x=0^+} = \int_0^a \frac{\tau(r_0)}{a^2}dr_0\int_0^a 2r\left[1+\sum_{n=1}^{\infty}\frac{J_0(k_nr_0)J_0(k_nr)}{J_0^2(k_na)}\right]dr = \int_0^a \tau(r_0)dr_0; \quad (37)$$

the transients [15] in the summation give zero contribution due to orthogonality of the constant function with $J_0(k_nr)$, see Eq. (A14). The function $\tau(r_0)$ and the difference C_b-C_a in Eq. (35) are scaled by the flux J. For the flat channel, $b=a$, the current density $j_x(0,r)$ is constant, so the flux flowing through the infinitesimal ring of radius r_0 is $\tau(r_0)=2r_0J/a^2$. If applied in Eq. (35), we get $C_b-C_a=0$ due to the same orthogonal relation. So in general, we expect

$C=(C_b-C_a)/J$ will play the same role as in the 2D channels.

Integrating $\rho(x,r)$ Eq. (34) over the cross section, we have

$$p(x) = \pi R^2 C_R - \mathrm{sgn}(x)\int_0^R 2\pi r dr \frac{|x|}{\pi R^2}\int_0^a \tau(r_0)dr_0 = \pi R^2 C_R - Jx. \quad (38)$$

Again, the transients in the sum of Eq. (36) give no contribution due to the orthogonality relations (A14). The resulting 1D density Eq. (38) represents free diffusion anywhere except at $x=0$, where it exhibits a jump. If $C_b=\rho_0$, which is fixed at the absorbing end of the channel, we arrive at a formula of the form Eq. (8),

$$p(x) = -J[x+\pi a^2 C\Theta(x)] + A(x)\rho_0, \quad (39)$$

$A(x)=\pi R^2(x)$.

The crucial constant $C=(C_b-C_a)/J$ is obtained by solving the integral equation (35) with use of the relation (37). For numerical solution, the formula (36) converges slowly; it can be replaced by Eq. (A25) in the Appendix.

IV. CONCLUSION

We examined mapping of diffusion in 2D and 3D channels with an abrupt change of diameter onto the longitudinal coordinate. Our analysis was based on direct calculation of the 2D (3D) stationary density $\rho(x,\mathbf{y})$. We used a conformal transformation in the complex plane for the 2D channels and then applied the method of sewing of solutions in the wide and narrow parts of the channel, which is also usable in 3D channels. The corresponding 1D density $p(x)$ Eq. (3) is unambiguously connected with the effective diffusion coefficient $D(x)$, entering the extended FJ Eq. (4), via the relation (7). As shown in Ref. [13], this method of determining $D(x)$ is equivalent to an exact mapping [6] in the limit of stationary flow, i.e., for slow processes.

Solution of the exactly solvable 2D channel demonstrated that although the abrupt change of width at $x=0$ influences the 2D density in a wide vicinity of this point, the stationary 1D density grows linearly everywhere except at the point of junction, where we observe a jump of $p(x)$. In the language of the effective diffusion coefficient $D(x)$, diffusion in such channels is free except of the point $x=0$. Here, the particles are diffusing along the transverse wall, and so their movement is invisible if viewed only in the longitudinal direction. Then the junction behaves like a trap. Let us stress that the trap is local, restricted to the point $x=0$ when the transverse relaxation is correctly taken into account.

The same picture is confirmed for symmetric 3D channels. The 1D description of such channels appears to be very simple. Aside from fixing the BCs at the ends, the relevant 1D diffusion is characterized only by one constant C, depending on the wider and narrower radii b and a, coming from the solution of the integral Eq. (35), or Eq. (26) for 2D channels. Unfortunately, they can be solved only numerically in general.

The method of sewing the solutions enables us to understand as well the reason that the 1D description is so simple here. The stationary density in the separated wide and narrow parts of the channels can be expressed explicitly as a sum of the transients [15], Eq. (36). Sewing of two halves of unequal diameters generates transients emanating from the junction (and decaying exponentially in distance $|x|$). Projection to 1D means integration over the cross section with the unit weight function, but here, the unit function is orthogonal to the transients. So they are integrated out in the 1D picture for $x\neq 0$. The remaining nonzero contribution has simplicity of the stationary flow in a flat channel.

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APPENDIX: DETAILED CALCULATIONS

We present here some details of calculation of the 2D density $\rho(x,y)$ using the conformal transformation for stepwise channels and then verification of the method of sewing by the exact solution for the 2D channel with the ratio $b/a=2$. Finally, we derive the Green's functions (23) for a flat 2D channel and $G_R(x,r|r_0)$ necessary for Eq. (34) in the 3D case.

The 2D density $\rho(x,y)$ in a stepwise channel [Fig. 1(b)] is given by the imaginary part of the complex function $h(w)$ Eq. (15), where $\chi(w)$ is the inverted transformation [Eq. (14)]. If we rewrite this relation in the form

$$e^{\sqrt{k}w} = \frac{z[2z-k-1+2\sqrt{(z-1)(z-k)}]^{\sqrt{k}}}{(k-1)^{\sqrt{k}-1}[(k+1)z-2k+2\sqrt{k(z-1)(z-k)}]}, \quad (A1)$$

we can find a substitution enabling us to convert it to a cubic or quartic equation for certain values of k and express the function $h(w)$ explicitly.

For $k=4$, corresponding to the widths $a=\pi/2$ and $b=\pi$, we substitute $\cosh Q=(2z-5)/3$. Then the Eq. (A1) becomes a cubic equation

$$e^{3Q}+3e^{2Q}-3e^{2w+Q}-e^{2w}=0, \quad (A2)$$

solvable by Cardano's formula,

$$e^Q = -1-\sqrt[3]{1+e^{2w}}(\sqrt[3]{1+ie^w}e^{i\nu}+\sqrt[3]{1-ie^w}e^{-i\nu}); \quad (A3)$$

$\nu=0,\pm 2\pi/3$ discerns three particular solutions. Taking care to choose the correct ν to make $\chi(w)$ consistent in the whole region of the channel and keeping $\mathrm{Re}[h(w)]=0$ and 1 at the lower and upper boundary, respectively, we arrive at $\chi(w)$ and finally $h(w)$ according to Eq. (15). Rotation of the complex plain $w=i\pi-s$, turning the channel to the desired position with the flat boundary identical with the x axis, also requires restoring the conditions (11) (they are flipped after the rotation). So the final $h(s)$ Eq. (16) is taken as $1-h(w=i\pi-s)$.

Next, verifying the method of sewing by the exact 2D solution for the ratio $b/a=2$, we start with the formula (16), containing the 2D density $\rho(x,y)$ in a 2D channel of the widths $b=\pi$ and $a=\pi/2$. As shown by the relation (27), the function $\tau(y)$ is proportional to the longitudinal current density $j_x(x,y)$ at $x=0^+$. It is effective to calculate it in the complex plane,

$$j_x(x,y) = -\operatorname{Im}\{\partial_x[\phi(x+iy)+i\rho(x+iy)]\} = -\operatorname{Im}[Jh'(z)]. \tag{A4}$$

From Eq. (16), we obtain

$$h'(z) = \frac{1}{\pi(1-i\sinh z)}\left[\cosh z + \frac{2i}{e^{2i\pi/3}r^{1/3}-r}\right], \tag{A5}$$

where $r=i\cosh z/(1-i\sinh z)$. Then

$$\operatorname{Im}[h'(z)|_{z=0^+ +iy}] = \frac{\sqrt{3}}{2\pi}\left[\sqrt[3]{\frac{\cos y}{(1+\sin y)}} + \sqrt[3]{\frac{(1+\sin y)}{\cos y}}\right], \tag{A6}$$

giving the formula (32) for $\tau(y)$.

Now, we need to verify that this function solves Eq. (26), i.e., if applied in this equation, the result of integration will not depend on y. It is convenient to substitute $u=\tan(y_0/2)$ and $v=\tan(y/2)$, transforming the left hand side integral to

$$I(v) = \frac{\sqrt{3}J}{2\pi^2}\int_{-1}^{1}\frac{du}{1+u^2}\left(\sqrt[3]{\frac{1-u}{1+u}} + \sqrt[3]{\frac{1+u}{1-u}}\right) \times \ln\left[\frac{16(1+uv)^2(u-v)^4}{(1+v^2)^3(1+u^2)^3}\right]. \tag{A7}$$

We check then the nullity of $dI(v)/dv$ [adopting the substitutions $p^3=(1+u)/(1-u)$ and $q^3=(1-v)/(1+v)$]. The resultant value of C_a-C_b can be calculated from Eq. (A7) taking an arbitrary v. Applying the same substitutions, we arrive at $C_a-C_b=(J/2\pi)\ln(2^8/3^9)$, yielding finally $C=(3/2\pi)\ln(27/16)$ from Eq. (31).

In the rest of this appendix, we derive the Eq. (23) and the 3D Green's function $G_R(x,r|r_0)$, used in Eq. (34).

The stationary density $\rho(x,y|y_0)$ around a pointlike source of particles placed at $(0,y_0)$ in a flat channel, bounded by $y=b$ and 0, (equivalent to the electrostatic potential around a charge placed in the same geometry with the dielectric walls) can be calculated by the method of mirrors [16]. Aside from the true source at $(0,y_0)$, we sum contributions to the density from all its mirror images with respect to the walls, lying at $y_m=y_0+2mb$ and $\bar{y}_m=-y_0+2mb$, m is an integer, to provide the Neumann BC at $y=0$ and b. To remove divergence of such a sum, we subtract the contributions of the mirror sinks, draining the particles at $(\pm 2L, y_m)$ and $(\pm 2L, \bar{y}_m)$ with the half strength of the sources at $x=0$. This guarantees zero density at $x=\pm L$ for large $L(\gg b)$. Adopting the well known logarithm formula for the potential of a single charge in the 2D plane, we write

$$\rho(x,y|y_o) = -Z\sum_{m=-\infty}^{\infty}\ln\frac{R_{0,m}^2\bar{R}_{0,m}^2}{R_{+,m}R_{-,m}\bar{R}_{+,m}\bar{R}_{-,m}}, \tag{A8}$$

$R_{0,m}=\sqrt{x^2+(y-y_m)^2}$, $R_{\pm,m}=\sqrt{(x\pm 2L)^2+(y-y_m)^2}$, $\bar{R}_{0,m}=\sqrt{x^2+(y-\bar{y}_m)^2}$, $\bar{R}_{\pm,m}=\sqrt{(x\pm 2L)^2+(y-\bar{y}_m)^2}$ and Z expresses the strength of the source. Summation of Eq. (A8) gives

$$\rho(x,y|y_0) = -\frac{Z}{2}\ln\frac{h_0^2(y_0)h_0^2(-y_0)}{h_+(y_0)h_-(y_0)h_+(-y_0)h_-(-y_0)}, \tag{A9}$$

where $h_\pm(y_0)=\cosh[\pi(2L\pm x)/b]-\cos[\pi(y-y_0)/b]$ and $h_0(y_0)=\cosh(\pi x/b)-\cos[\pi(y-y_0)/b]$. The functions

$$\ln h_\pm(y_0) = \frac{\pi}{b}(2L\pm x) - \ln 2 + \ln\left(1 - 2\cos\frac{\pi(y-y_0)}{b} \times e^{-\pi(2L\pm x)/b} + e^{-2\pi(2L\pm x)/b}\right) \tag{A10}$$

become constants (proportional to L) in the limit $L\to\infty$, as the exponential terms in Eq. (A10) become negligible. The denominator in Eq. (A9) can be hidden in the integration constant C_L. Thus we arrive at the Eq. (23). The strength of the source Z is replaced by the net flux J flowing through the (positive) part of the channel.

The 3D Green's function $G_R(x,r|r_0)$ in Eq. (34) is related to the stationary density generated by a ring source of particles of radius r_0, placed symmetrically in the cylinder of radius R at $x=0$. Outside the source, the 3D density $\rho(x,r)$ (not depending on the angle ϕ due to the symmetry) satisfies the equation

$$[(1/r)\partial_r r\partial_r + \partial_x^2]\rho(x,r) = 0, \tag{A11}$$

which is separable. Its particular solutions $e^{-k|x|}J_0(kr)$ (J_0 denotes the Bessel function) provide the expected decay for growing $|x|$, as well as nonsingular behavior at $r=0$. The parameter $k>0$ is fixed to satisfy the Neumann BC at $r=R$. So the density has the form

$$\rho(x,r) = -c_0|x| + \rho_0 + \sum_{n=1}^{\infty} c_n e^{-k_n|x|}J_0(k_n r), \tag{A12}$$

n enumerates the roots of $J_1(k_nR)=0$, ρ_0 is fixed at the distant absorbing end of the channel. The coefficients c_n have to ensure that the longitudinal flux $j_x(x,r)$ at $x=0^+$ is proportional to $\delta(r-r_0)$; the integral of $j_x(x,r)$ around the source ring is

$$2\pi r j_x(0^+,y) = 2\pi r\left[c_0 + \sum_{n=1}^{\infty} c_n k_n J_0(k_n r)\right] = J\delta(r-r_0). \tag{A13}$$

Applying the orthogonality relations for Bessel functions [17],

$$\int_0^R rJ_0(k_n r)dr = 0,$$

$$\int_0^R rJ_0(k_n r)J_0(k_m r)dr = \frac{R^2}{2}J_0^2(k_n R)\delta_{n,m}, \tag{A14}$$

we obtain

$$\rho(x,r) = \frac{J}{\pi R^2}\left[-|x| + \sum_{n=1}^{\infty} e^{-k_n|x|}\frac{J_0(k_n r_0)J_0(k_n r)}{k_n J_0^2(k_n R)}\right]. \tag{A15}$$

The function $G_R(x,r|r_0)$ in Eq. (36) is the 3D density [Eq. (A15)] for the unit flux.

The sum in Eq. (A15) converges slowly and so it is not suitable for numerical solving of Eq. (35). Instead, we derive an alternative formula.

The 3D Green's function G_{3D}, corresponding to a point like source, satisfies the equation

$$\left(\frac{1}{r}\partial_r r\partial_r + \frac{1}{r^2}\partial_\phi^2 + \partial_x^2\right)G_{3D}(\vec{r},\vec{r}') = -\frac{1}{r}\delta(x-x')\delta(r-r')\delta(\phi-\phi') \tag{A16}$$

in cylindrical coordinates [18]. The axial symmetry of the source, as well as of the resultant density, enables us to integrate G_{3D} and Eq. (A16) over the angle ϕ' (over the length of the source ring),

$$G(x,r|x',r') = 2\pi r' G_{3D}(\vec{r},\vec{r}'),$$

$$\left[\frac{1}{r}\partial_r r\partial_r - \partial_x^2\right]G(x,r|x',r') = -\delta(r-r')\delta(x-x'). \tag{A17}$$

To handle a singularity appearing in this calculation, we suppose first a finite cylinder, $|x|<L$ with the source ring placed at $x'=0$ and both ends at $x=\pm L$ absorbing. So $G(x,r|0,r')=G(x,r|r')$ becomes a periodic function with the period $4L$ and we can perform the Fourier transform,

$$G(x,r|r') = \frac{1}{L}\sum_k G_k(r|r')\cos kx,$$

$$\left[\frac{1}{r}\partial_r r\partial_r - k^2\right]G_k(r|r') = -\delta(r-r'), \tag{A18}$$

k runs over $(n+1/2)\pi/L$, $n=0,1,\ldots$. The last equation is solved using the solutions $\psi_\pm(r)$ of the homogeneous equation

$$\left[\frac{1}{r}\partial_r r\partial_r - k^2\right]\psi_\pm(r) = 0, \tag{A19}$$

satisfying desired BCs on the left and right boundaries. The particular solutions of Eq. (A19) are the Bessel functions $I_0(kr)$ and $K_0(kr)$. The density at $r=0$ has to be finite, hence $\psi_-(r)$ cannot contain $K_0(kr)$. The upper solution, $\psi_+(r)=I_0(kr)+\alpha_k K_0(kr)$, satisfies the Neumann BC $\partial_r\psi_+(x)|_{r=R}=0$, which fixes α_k, so

$$\psi_-(r) = I_0(kr), \quad \psi_+(r) = I_0(kr) + \frac{I_1(kR)}{K_1(kR)}K_0(kr). \tag{A20}$$

Then $G_k(r|r')=-\psi_+(r_>)\psi_-(r_<)/W$; $r_>$ is the maximum and $r_<$ the minimum of $\{r,r'\}$. The Wronskian $W=\psi_+'(r)\psi_-(r)-\psi_-'(r)\psi_+(r)=-I_1(kR)/rK_1(kR)$. Taking $\delta(r-r')=(r'/r)\delta(r-r')$ into account, hidden in Eqs. (A17) and (A18), the calculation results in

$$G_k(r|r') = r' I_0(kr_<)\left[K_0(kr_>) + \frac{K_1(kR)}{I_1(kR)}I_0(kr_>)\right]. \tag{A21}$$

The first term does not depend on R and so it corresponds to the density generated by the source ring of radius r' in an unbounded space. If $L\to\infty$, the summation in Eq. (A18) becomes integration,

$$G_\infty(x,r|r') = \frac{r'}{\pi}\int_0^\infty I_0(kr_<)K_0(kr_>)\cos(kx)dk = \frac{r'}{\pi\sqrt{x^2+(r+r')^2}}\mathbf{K}\left(\frac{2\sqrt{rr'}}{\sqrt{x^2+(r+r')^2}}\right), \tag{A22}$$

where $\mathbf{K}(z)$ denotes the complete elliptic integral [17]. The same formula describes the electrostatic potential generated by the same ring charged by the charge $2\pi r'$.

The second part of Eq. (A21) diverges for $k\to 0$,

$$I_0(kr)I_0(kr')\frac{K_1(kR)}{I_1(kR)} \simeq \frac{2}{kR}\left(\frac{1}{kR} + \frac{kR}{2}\ln\frac{kR}{2} + \cdots\right). \tag{A23}$$

The diverging leading term is connected with the Fourier transform of the function $L-|x|$ for $|x|<2L$, repeated with period $4L$,

$$L - |x| = \sum_{n=0}^{\infty}\frac{8L}{(2n+1)^2\pi^2}\cos\left[\left(n+\frac{1}{2}\right)\frac{\pi x}{L}\right], \tag{A24}$$

so we obtain the contribution $r'(L-|x|)/R^2$ to $G(x,r|r')$ Eq. (A18) from it. We can omit the diverging constant $\sim L$ and replace the remaining sum by integration over k in the limit $L\to\infty$. Finally, the resulting formula

$$G_R(x,r|r') = -\frac{|x|}{\pi R^2} - \frac{1}{\pi^2}\int_0^\infty\left[\frac{2}{(kR)^2} - I_0(kr)I_0(kr')\frac{K_1(kR)}{I_1(kR)}\right]\cos(kx)dk + \frac{1}{\pi^2\sqrt{x^2+(r+r')^2}}\mathbf{K}\left(\frac{2\sqrt{rr'}}{\sqrt{x^2+(r+r')^2}}\right) \tag{A25}$$

is multiplied by 2, because the particles are emitted only into a half (left or right) of the cylinder in our consideration, and also divided by $2\pi r'$, introduced at the beginning by integration of $G_{3D}(\vec{r},\vec{r}')$ over the length of the source ring. This factor is already included in our definition of the function $\tau(r_0)$, Eq. (34). One can check numerically the equivalence of this formula with Eq. (36).

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