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Mapping of forced diffusion in quasi-one-dimensional systems

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Diffusion in an external potential in a two-dimensional channel of varying cross section is considered. We show that a rigorous mapping procedure applied on the corresponding Smoluchowski equation yields a one-dimensional evolution equation of the Fick-Jacobs type corrected by an effective coefficient $D(x)$. The procedure enables us to derive this function within a recurrence scheme. We test this result on a model of stationary diffusion in a linear cone in a homogeneous potential, which is exactly solvable. Extension of the approximate formulas for $D(x)$ derived for the diffusion alone is discussed.

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I. INTRODUCTION

Understanding classical transport in nanomaterials or biological systems, which are of an increasing interest in the last decade, usually requires to solve the Fokker-Planck equation in narrow nonhomogeneous channels. Instead of solving the full-dimensional problem, one can look first for a certain kind of dimensional reduction in the equation, and then to deal with a low-dimensional [or one-dimensional (1D)] problem only, giving us a higher chance to find the solution in a concise form.

The best understood case is the simplest one: diffusion in a channel with varying cross section $A(x)$; x denotes the longitudinal coordinate. The d-dimensional diffusion equation,

$$\frac{\partial\rho(x,\mathbf{y},t)}{\partial t}=\left[D_0\frac{\partial^2}{\partial x^2}+D_y\sum_{j=1}^{d-1}\frac{\partial^2}{\partial y_j^2}\right]\rho(x,\mathbf{y},t), \qquad (1.1)$$

in the channel with reflecting boundaries can be reduced to the Fick-Jacobs (FJ) equation [1],

$$\frac{\partial p(x,t)}{\partial t}=D_0\frac{\partial}{\partial x}A(x)\frac{\partial}{\partial x}\frac{p(x,t)}{A(x)}, \qquad (1.2)$$

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

$$p(x,t)=\int_{A(x)}\rho(x,\mathbf{y},t)d\mathbf{y}, \qquad (1.3)$$

the integral of the d-dimensional density $\rho(x,\mathbf{y},t)$ over the transverse coordinates $\mathbf{y}=(y_1,\ldots,y_{d-1})$; $D_0=D_y$ is the diffusion constant.

The next studies [2,3] showed that Eq. (1.2) is too simple, giving unsatisfactory results in several cases. Reguera and Rubí [3] proposed to correct the FJ equation by a function $D(x)$,

$$\frac{\partial p(x,t)}{\partial t}=\frac{\partial}{\partial x}A(x)D(x)\frac{\partial}{\partial x}\frac{p(x,t)}{A(x)}, \qquad (1.4)$$

an effective diffusion coefficient estimated by the formula

$$D(x)=D_0[1+R'^2(x)]^{-\eta_d}, \qquad (1.5)$$

based on heuristic arguments. In two dimensions (2D), $R(x)=A(x)$ is the width of the channel and $\eta_2=1/3$; for three-dimensional (3D) symmetric channels, $R(x)$ denotes the x-dependent radius, $A(x)=\pi R^2(x)$, and $\eta_3=1/2$.

The projection technique [4,5] based on introducing anisotropy of the diffusion constant $D_y=D_0/\epsilon>D_0$ in Eq. (1.1) and the reflecting boundary conditions (BCs), which is equivalent to scaling of the transverse lengths $[y_i,A(x),R(x),\ldots]$ by $\sqrt{\epsilon}$, enabled us to separate the fast transverse modes (transients) from the slow longitudinal ones in d-dimensional systems and to project them out by integration over the cross section. The result is a recurrence scheme, generating systematically corrections to the FJ equation as an expansion in ϵ, starting with the right-hand side of Eq. (1.2) as the lowest-order term.

In the limit of the stationary flow, the corrected FJ equation coming from this procedure takes the form of Eq. (1.4) and the recurrence scheme enables us to fix $D(x)$ unambiguously as an expansion in ϵ [6]. If the second and higher derivatives of $A(x)$ or $R(x)$ are neglected, $D(x)$ becomes summable. For the symmetric 3D channels, the formula (1.5) is recovered in the limit $\epsilon\to 1$. Summation in the 2D case gives

$$D(x)=D_0\frac{\arctan A'(x)}{A'(x)}, \qquad (1.6)$$

which differs only slightly from the estimate (1.5) for $|A'|<1$, so both formulas are still used. Usability of Eq. (1.5) was tested numerically [7] and including the higher derivatives of $A(x)$ in $D(x)$ was discussed in Ref. [8].

However, aside from the diffusion, the particles are also driven by forces in real systems. The simplest way of studying such models of the narrow channels is introducing an "entropic" potential $U_{ent}(x)$. The cross-section area $A(x)$ is represented as a Boltzmann weight $\exp[-\beta U_{ent}(x)]$; $\beta=1/k_BT$ denotes the inverse temperature, and $U_{ent}(x)$ is simply added to the "real" potential $U(x)$, entering the evolution (Smoluchowski) equation. Again, the equation, or the corresponding solution can be corrected by an effective coefficient $D(x)$; the formula (1.5) (derived for the pure diffusion) was usually applied in this case [9–13].

For periodic channels, the effective mobility μ_{eff} and the diffusion coefficient D_{eff} can be defined meaningfully by using the large time limit of the mean velocity $\langle\dot{x}(t)\rangle$ and the variance of the position $x(t)$ of a particle inserted in the channel [14]. These quantities can be computed by Brownian dynamic simulations, as well as calculated from the first two moments of the first passage time [10,12] determined from the 1D evolution equation. Comparison of the results for the sinusoidal 2D channel with a constant force obtained by both methods showed [12] that including the correcting coefficient (1.5) works well but only for small forces.

For calculation of the mean velocity and dispersivity (D_{eff}) in periodic channels, the macrotransport theory [15,16] was successfully applied. Starting from the Smoluchowski equation with reflecting BC and adopting the scaling of the transverse lengths by ϵ (corresponding to $\sqrt{\epsilon}$ in our mapping), the moments of the 1D density $p(x,t)$ were expressed rigorously as an expansion in ϵ^2. This theory exhibited good agreement with numerical simulations in the whole range of the applied forces.

The aim of the present paper is to demonstrate that also the 1D evolution equation for the forced diffusion can be derived rigorously by mapping of the Smoluchowski equation. If the force acts in the x direction, the potential $U(x)$ does not depend on the transverse coordinates and the anisotropy of the diffusion constant (scaling of the transverse lengths) can be introduced. Then the mapping procedure can be applied in the same way as for the diffusion alone. We arrive at the equation

$$\frac{\partial p(x,t)}{\partial t} = \frac{\partial}{\partial x}A(x)D(x)e^{-\beta U(x)}\frac{\partial}{\partial x}e^{\beta U(x)}\frac{p(x,t)}{A(x)} \qquad (1.7)$$

valid in the limit of the stationary flow; the effective coefficient $D(x)$ is expressed consistently as an expansion in $\epsilon = D_0/D_y$ and depends not only on the derivatives of $A(x)$ but also of $U(x)$. The mapping does not require periodicity of the channel or the force; $A(x)$ and $U(x)$ should be analytic functions.

The mapping procedure is presented in the following section. In Sec. III, we test the resultant $D(x)$ on a linear cone with a constant force, which is an exactly solvable model. Finally, we discuss possibility of extending the formula (1.6) to diffusion under a constant force.

For simplicity, the mapping will be carried out only for 2D channels; its extension to higher-dimensional geometries (e.g., symmetric 3D channels) is straightforward.

II. MAPPING PROCEDURE

We consider a 2D channel bounded by x axis and an analytic function $A(x) > y > 0$. Diffusing particles are dragged by a force along the x axis; hence, the potential $U(x)$ in the channel depends only on the x coordinate. Then the 2D density $\rho(x,y,t)$ obeys the Smoluchowski equation,

$$\frac{\partial \rho(x,y,t)}{\partial t} = D_0\frac{\partial}{\partial x}W(x)\frac{\partial}{\partial x}\frac{\rho(x,y,t)}{W(x)} + \frac{D_0}{\epsilon}\frac{\partial^2 \rho(x,y,t)}{\partial y^2}, \qquad (2.1)$$

where $W(x)=\exp[-\beta U(x)]$; we put $D_0=1$ in our next considerations. As used in the mapping of the diffusion alone [4], we introduce here anisotropy of the diffusion constant; the diffusion in the transverse direction is supposed $1/\epsilon$ times faster. This enables us to separate the transients in the transverse direction, which are to be integrated out [5]. In our mapping procedure, $\epsilon \in (0,1)$ serves as a small parameter, in which the spatial operator of the mapped equation is expanded.

The Smoluchowski equation (2.1) represents the mass conservation law, so the components of the current density $\mathbf{j}$ are

$$j_x(x,y,t) = -W(x)\partial_x[\rho(x,y,t)/W(x)],$$

$$j_y(x,y,t) = -(1/\epsilon)\partial_y \rho(x,y,t). \qquad (2.2)$$

The vector $\mathbf{j}$ at the boundaries has to be parallel with them; this requirement gives the Neumann BCs

$$\partial_y \rho(x,y,t) = 0|_{y=0},$$

$$\partial_y \rho(x,y,t) = \epsilon A'(x)W(x)\partial_x \left.\frac{\rho(x,y,t)}{W(x)}\right|_{y=A(x)}. \qquad (2.3)$$

The first step of the mapping is to integrate Eq. (2.1) over the local cross section. Completing double integration by parts and using BC (2.3), we arrive at the equation

$$\frac{\partial p(x,t)}{\partial t} = \frac{\partial}{\partial x}W(x)\frac{\partial}{\partial x}\frac{p(x,t)}{W(x)} - \frac{\partial}{\partial x}[A'(x)\rho(x,A(x),t)], \qquad (2.4)$$

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

$$p(x,t) = \int_0^{A(x)} \rho(x,y,t)dy. \qquad (2.5)$$

The crucial point of the mapping procedure is to express the 2D density at the upper boundary $\rho[x,A(x),t]$ in Eq. (2.4) by using the 1D density $p(x,t)$. We start with the case $\epsilon \to 0$, when the transverse diffusion constant $D_0/\epsilon \to \infty$. The relaxation in the y direction is infinitely fast; hence, the transverse profile of the 2D density remains flat; $\rho(x,y,t) = p(x,t)/A(x)$ to satisfy the normalization condition (2.5). If substituted in Eq. (2.4), we get

$$\frac{\partial p(x,t)}{\partial t} = \frac{\partial}{\partial x}\left[W(x)\frac{\partial}{\partial x}\frac{p(x,t)}{A(x)} - \frac{A'(x)}{A(x)}p(x,t)\right]$$
$$= \frac{\partial}{\partial x}A(x)W(x)\frac{\partial}{\partial x}\frac{p(x,t)}{A(x)W(x)}, \qquad (2.6)$$

which is equivalent to the FJ equation.

For $\epsilon > 0$, we can derive a recurrence procedure generating a sequence of corrections to the spatial operator of Eq. (2.6). The most effective way is to look for an operator $\hat{\omega}(x,y,\partial_x)$, mapping the 1D density $p(x,t)$ back to the space of solutions of the original 2D Smoluchowski equation (2.1), in the form of a series in ϵ

$$\rho(x,y,t) = W(x)\hat{\omega}(x,y,\partial_x)\frac{p(x,t)}{A(x)W(x)} = W(x)\sum_{j=0}^{\infty}\epsilon^j\hat{\omega}_j(x,y,\partial_x)\frac{p(x,t)}{A(x)W(x)}. \tag{2.7}$$

Fixing $\hat{\omega}_0=1$ restores the Eq. (2.6) in the order ϵ^0. If it is substituted for ρ in Eq. (2.1), we get

$$\sum_{j=0}^{\infty}\epsilon^j\left[\partial_t - \partial_x W(x)\partial_x\frac{1}{W(x)} - \frac{1}{\epsilon}\partial_y^2\right]W(x)\hat{\omega}_j(x,y,\partial_x)\frac{p(x,t)}{A(x)W(x)} = 0. \tag{2.8}$$

The time derivative ∂_t commutes with the spatial operators and for $\partial_t p(x,t)$, we use the mapped equation expected in the form

$$\partial_t p(x,t) = \partial_x A(x)W(x)[1-\epsilon\hat{Z}(x,\partial_x)]\partial_x\frac{p(x,t)}{A(x)W(x)}, \tag{2.9}$$

where the unknown operator $\hat{Z}(x,\partial_x)$ is also expanded

$$\epsilon\hat{Z}(x,\partial_x) = \sum_{k=1}^{\infty}\epsilon^k\hat{Z}_k(x,\partial_x). \tag{2.10}$$

Combining Eqs. (2.8)–(2.10) and comparing the coefficients at ϵ^j, we get the recurrence relation

$$\partial_y^2\hat{\omega}_{j+1}(x,y,\partial_x) = -\frac{1}{W(x)}\partial_x W(x)\partial_x\hat{\omega}_j(x,y,\partial_x) - \sum_{k=0}^{j}\hat{\omega}_{j-k}(x,y,\partial_x)\frac{1}{A(x)W(x)} \times\partial_x A(x)W(x)\hat{Z}_k(x,\partial_x)\partial_x, \tag{2.11}$$

we take $\hat{Z}_0(x,\partial_x)=-1$ in this formula. After double integration of $\partial_y^2\hat{\omega}_{j+1}$, we fix two integration constants to satisfy BC (2.3) and the normalization condition,

$$\int_0^{A(x)} dy\,\hat{\omega}_j(x,y,\partial_x) = 0, \tag{2.12}$$

for $j>0$, coming from Eq. (2.5). Finally, the corresponding operator $\hat{Z}_j(x,\partial_x)$ is obtained from Eq. (2.4), if the jth order term of the 2D density at the boundary $\rho[x,A(x),t]$ in ϵ is expressed by the backward mapped $p(x,t)$ onto the space of 2D solutions of the original Smoluchowski equation (2.1), i.e., by using Eq. (2.7) with the operator $\hat{\omega}_j(x,y,\partial_x)$ taken at $y=A(x)$. After comparison with Eq. (2.9), we find

$$\hat{Z}_j(x,\partial_x)\partial_x = \frac{A'(x)}{A(x)}\hat{\omega}_j[x,A(x),\partial_x] \quad \text{for} \quad j>0. \tag{2.13}$$

This scheme enables us to calculate simultaneously $\hat{\omega}_j$ and $\hat{Z}_j$ up to an arbitrary order, starting from $\hat{\omega}_0=1$ and $\hat{Z}_0=-1$, representing the FJ equation (2.6). The resulting expansion of $\hat{\omega}$ reads as

$$\hat{\omega}(x,y,\partial_x) = 1 + \frac{\epsilon A'(x)}{6A(x)}[3y^2 - A^2(x)]\partial_x + \ldots, \tag{2.14}$$

the second- and the higher-order terms in ϵ contain also derivatives of the potential $U(x)$. Then the mapped equation up to the second order is

$$\partial_t p(x,t) = \partial_x AW\left\{1 - \frac{\epsilon}{3}A'^2 - \frac{\epsilon^2 A'}{45}[2A(AA')'\partial_x + A^2A^{(3)} + AA'A'' - 7A'^3 + \beta A(A'^2U' + AA'U'' - AA''U')] + \ldots\right\}\partial_x\frac{p(x,t)}{AW}. \tag{2.15}$$

The resultant spatial operator on the right-hand side of this equation contains the derivatives ∂_x up to the $j+1$st order in the ϵ^j term and it is too complicated for use in practice. The mapped equation becomes simpler in the stationary regime. Like in the mapping of the diffusion equation [6], the operator $[1-\epsilon\hat{Z}]$ can be replaced by a function $D(x)$ in the limit of stationary flow; the mapped equation can be rewritten in the form

$$\frac{\partial p(x,t)}{\partial t} = \partial_x A(x)W(x)D(x)\partial_x\frac{p(x,t)}{A(x)W(x)}. \tag{2.16}$$

Both Eqs. (2.15) and (2.16) represent the 1D mass conservation law, so the 1D flux $J(x,t)$ can be expressed as

$$J(x,t) = -\int_0^{A(x)}\partial_x\rho(x,y,t)dy = -A(x)W(x)D(x)\partial_x\frac{p(x,t)}{A(x)W(x)}, \tag{2.17}$$

from Eq. (2.16) and

$$J(x,t) = -A(x)W(x)[1-\epsilon\hat{Z}(x,\partial_x)]\partial_x\frac{p(x,t)}{A(x)W(x)}, \tag{2.18}$$

from Eq. (2.15). In the stationary regime, the flux $J(x,t)=J$ is constant in x and t, and a relation between $D(x)$ and $\hat{Z}(x,\partial_x)$ can be found. For a given flux J, the derivative $\partial_x[p(x)/A(x)W(x)]=-J/A(x)W(x)D(x)$, as expressed from Eq. (2.17), becomes a function depending only on geometry of the channel and the potential $U(x)$. If substituted in Eq. (2.18), we get after simple algebra

$$\frac{1}{D(x)} = A(x)W(x)[1-\epsilon\hat{Z}(x,\partial_x)]^{-1}\frac{1}{A(x)W(x)}, \tag{2.19}$$

which fixes the effective diffusion coefficient $D(x)$ unambiguously for $\hat{Z}$ obtained from the mapping procedure. For $\hat{Z}$ in 2D channels, contained in Eq. (2.15), we obtain

$$D(x) = 1 - \frac{\epsilon}{3}A'^2 + \frac{\epsilon^2 A'}{45}[9A'^3 + AA'A'' - A^2A^{(3)} - \beta A(3A'^2U' + AA''U' + AA'U'')] + \ldots. \tag{2.20}$$

Formula (2.16) for J can be rewritten in a more standard form

$$J(x,t) = -D(x)\left[A(x)\partial_x \frac{p(x,t)}{A(x)} + \beta U'(x)p(x,t)\right], \tag{2.21}$$

where the diffusion and the mobility terms are separated. The effective function $D(x)$ corrects both, mobility and the diffusion constant in the same way, keeping (a kind of) the Einstein relation between them valid.

The mapping presented shows that the concept of the entropic potential works only within the FJ approximation, i.e., if the relaxation in the transverse directions is considered infinitely fast. In Eq. (2.6), $A(x)$ and $W(x)$ are combined in the product, which enables us to understand $A(x)$ as a Boltzmann factor $\exp[-\beta U_{ent}(x)]$. Then the "entropic" potential $U_{ent}(x)$ can be simple added to the real potential $U(x)$. This is no more valid if the next corrections are included; the contributions from the derivatives of $A(x)$ and $U(x)$ enter the effective coefficient $D(x)$ in various different combinations.

Extension of the mapping to more complicated geometries of the channels is straightforward. The form of the mapped Eq. (2.9) remains the same; the operator $\hat{Z}$ depends on dimensionality and symmetry of the channel. For 3D channels with cylindrical symmetry, we find

$$\partial_t p(x,t) = \partial_x A(x)W(x)\Big\{1 - \frac{\epsilon}{2}R'^2 - \frac{\epsilon^2 R'}{48}[2R(RR')'\partial_x + R^2R^{(3)} + RR'R'' - 14R'^3 + \beta R(R'^2U' - RR''U' + RR'U'')] - \dots\Big\}\partial_x \frac{p(x,t)}{A(x)W(x)}, \tag{2.22}$$

R denotes the local radius $R(x)$ and $A(x)=\pi R^2(x)$ here. In the stationary regime, we obtain

$$D(x) = 1 - \frac{\epsilon}{2}R'^2 + \frac{\epsilon^2 R'}{48}[18R'^3 + 3RR'R'' - R^2R^{(3)} - \beta R(3R'^2U' + RR''U' + RR'U'')] - \dots \tag{2.23}$$

One can easily check that in the limit $U(x)=\text{const}$, formulas (2.20) and (2.23) restore $D(x)$ known for the diffusion alone [6].

III. EXACT MODEL

In this section, we present the solution of an exactly solvable model: the stationary flow of particles diffusing in a linear cone bounded by $y=A(x)=\alpha x$ and the x axis and dragged by a constant force F in x direction. We calculate the corresponding function $D(x)$, check the expansion (2.20), and discuss possibility of extension of the approximation (1.6) for nonzero force.

The solution is trivial for zero force [8]. If we suppose a pointlike source of particles at the origin of the coordinate system, the model has radial symmetry. Then the density $\rho(x,y)=-C\ln[(x^2+y^2)/l_0^2]$ satisfies the stationary diffusion equation $(\partial_x^2+\partial_y^2)\rho=0$, valid outside the source. The lines $y=\alpha x$ of any α are parallel to the current density $\mathbf{j}=-\nabla\rho$, so the "no flux" BC at these lines is satisfied too. The integration constant C is fixed to set the correct flux J flowing through the cone $0<y<\alpha x$; the constant l_0, adjusting BC $\rho(x,y)=0$ at the distance l_0 from the source, is irrelevant in calculation of $D(x)$ [8].

A nonzero force parallel to the x axis breaks the radial symmetry and the solution is not so easy. Still, the Smoluchowski equation (2.1) can be symmetrized for the corresponding potential $U(x)=-Fx$ by the substitution

$$\rho(x,y) = e^{\beta Fx/2}u(x,y), \tag{3.1}$$

then the stationary equation in the polar coordinates (r,ϕ) reads as

$$\left[\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2} - \left(\frac{\beta F}{2}\right)^2\right]u(r,\phi) = 0, \tag{3.2}$$

for $r>0$ (outside the source) and $\epsilon=1$. This equation is separable; $u(r,\phi)=R_\nu(r)\cos\nu\phi$ and the solutions for the radial part $R_\nu(r)$ are the Bessel functions $I_\nu(\beta Fr/2)$ and $K_\nu(\beta Fr/2)$.

The functions I_ν diverge in $r\to\infty$, so they cannot be contained in the solution for the unbounded plain. In this case, the stationary regime is described by the density

$$\rho_0(x,y) = Ce^{\beta Fx/2}K_0\left(\frac{\beta F}{2}\sqrt{x^2+y^2}\right), \tag{3.3}$$

which carries the 1D flux J flowing for $x>0$

$$J = -\int_{-\infty}^{\infty} dy e^{\beta Fx}[\partial_x e^{-\beta Fx}\rho_0(x,y)] = 2\pi C. \tag{3.4}$$

In the region of small βFr, the leading term of $\rho_0 \sim \ln r$, so the homogeneous diffusion from the pointlike source is dominant near the source. Using the asymptotic expansion of K_0 [17] for large βFr, we get

$$\rho_0(x,y) \sim (x^2+y^2)^{-1/4}e^{-\beta F(\sqrt{x^2+y^2}-x)/2}, \tag{3.5}$$

which is nearly the Gaussian in y with $\langle y^2\rangle \simeq 2x/\beta F$. This corresponds to the expected large scale picture; the particles diffuse in y direction ($D_0=1$) and move in x direction from the source with the mean velocity βF.

Nevertheless, the density (3.3) does not satisfy the BC (2.3) on any line $y=\alpha x$ except of $\alpha=0$. To find a solution satisfying the BC for a specific α, one can consider adding a linear combination of other $K_\nu(\beta Fr/2)\cos\nu\phi$ in $u(r,\phi)$. If we represent the Bessel functions K_ν by the integral [17],

$$K_\nu(r) = \int_0^\infty e^{-r\cosh t}\cosh\nu t dt, \tag{3.6}$$

then any solution of Eq. (3.2) based on K_ν has the form

$$u(r,\phi) = \int_0^\infty e^{-(\beta Fr/2)\cosh t}[f(t+i\phi)+f(t-i\phi)]dt, \tag{3.7}$$

$f(z)$ is some analytic function of the complex variable z. Applying Eq. (3.7) in Eq. (3.2) and performing double integration by parts, we find that any $f(z)$ satisfying the condition $[f'(t+i\phi)+f'(t-i\phi)]|_{t=0}=0$ for any ϕ generates a solution of Eq. (3.2).

Finally, we fix the BC at the boundary $y=\alpha x$. In the polar coordinates, $0<\phi<\phi_0$, where $\alpha=\tan\phi_0$, the BC (2.3) for $u(r,\phi)$ becomes

$$\partial_\phi u(r,\phi)|_{\phi=\phi_0} = -\sin\phi_0\left(\frac{\beta F r}{2}\right)u(r,\phi_0) \quad (3.8)$$

for any radius r; BC at the x axis $\partial_\phi u(r,\phi)|_{\phi=0}=0$ is satisfied by the symmetry. If Eq. (3.7) is used in Eq. (3.8), we arrive at the conditions $f(i\phi_0)=f(-i\phi_0)$ and

$$[f(t+i\phi_0)-f(t-i\phi_0)]\sinh t = i[f(t+i\phi_0)+f(t-i\phi_0)]\sin\phi_0 \quad (3.9)$$

for any $t\in(0,\infty)$. The last one is satisfied if $f(z)=g(z)\tanh(z/2)$ and $g(z)$ fulfills the relation $g(t+i\phi_0)=g(t-i\phi_0)$ for any t. The important solution is generated by $g_0(z)=\coth(\pi z/2\phi_0)$. We show in the Appendix that it is connected with the 1D stationary flux

$$J=-\int_0^{\alpha x} dy e^{\beta F x}[\partial_x e^{-\beta F x/2}u(x,y)] = 2\phi_0, \quad (3.10)$$

flowing along the x axis. The other solutions generated by $g_n(z)=\sinh(n\pi z/\phi_0)$; $n=1,2,\ldots$ are the transients not carrying the longitudinal flux and projected out by the mapping procedure. For integer π/ϕ_0, these solutions can be integrated from Eq. (3.7); e.g., if $\phi_0=\pi/3$, $g_1(z)$ generates $u(r,\phi)$ proportional to

$$K_0(\tilde r)-2K_1(\tilde r)\cos\phi+2K_2(\tilde r)\cos 2\phi-K_3(\tilde r)\cos 3\phi,$$

$\tilde r=\beta F r/2$, but the solution (3.7) with

$$f(z)=g_0(z)\tanh\left(\frac{z}{2}\right)=\coth\left(\frac{\pi z}{2\phi_0}\right)\tanh\left(\frac{z}{2}\right), \quad (3.11)$$

which is of our interest, has to be treated in its integral form in the next calculations.

Having calculated the stationary 2D density $\rho(x,y)$, we can express the effective diffusion constant $D(x)$ from the formula (2.17)

$$\frac{J}{D(x)} = -x e^{\beta F x}\partial_x\left[\frac{1}{x}e^{-\beta F x}\int_0^{\alpha x}\rho(x,y)dy\right]. \quad (3.12)$$

After some algebra (see the Appendix), we arrive at the final formula

$$\frac{1}{D(x)} = 1+\frac{1}{\beta F x}-\frac{2\pi\alpha}{\beta F x\phi_0^2} \times\int_0^\infty \frac{dt}{[1+\cosh(\pi t/\phi_0)]}\frac{\cos\phi_0}{(\cosh t+\cos\phi_0)} \times\exp\left(-\frac{\beta F x}{2}\left[\frac{\cosh t}{\cos\phi_0}-1\right]\right). \quad (3.13)$$

The integrals in Eqs. (3.7) and (3.13) converge only for $Fx\geq 0$. For negative Fx, the integration path in both formulas has to be changed

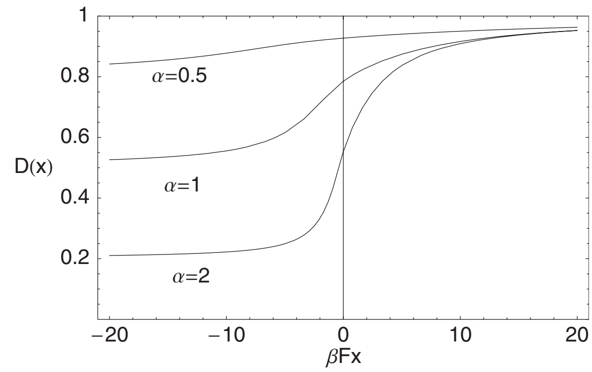

FIG. 1. Effective diffusion coefficient $D(x)$ for the linear cone bounded by $y=\alpha x$ and the x axis with a constant force F acting in the x direction.

$$\int_0^\infty dt\ldots \to \frac{1}{2}\left(\int_0^{\infty+i\pi} dt\ldots + \int_0^{\infty-i\pi} dt\ldots\right),$$

the path is arbitrary, but avoiding the poles on the imaginary axis from the right side (Fig. 7). The corresponding details are given in the Appendix.

The coefficients of the expansion of the integral in Eq. (3.13) in $\beta F x$ can be expressed explicitly (shown in the Appendix); we get

$$\frac{1}{D(x)} = 1+\frac{1}{\beta F x}-\frac{1}{\beta F x}e^{\beta F x}\left[1-\frac{\alpha\beta F x}{\phi_0}+\frac{\alpha(\beta F x)^2}{4\phi_0} \times\left(1+\frac{2\phi_0}{\sin 2\phi_0}\right)-\ldots\right]. \quad (3.14)$$

Taking $\phi_0=\arctan\alpha$, the expansion of $D(x)$ in $\beta F x$ and α yields

$$D(x)=\frac{\arctan\alpha}{\alpha}+\beta F x\left(\frac{\alpha^4}{15}-\frac{5\alpha^6}{63}+\frac{2\alpha^8}{25}-\ldots\right) +(\beta F x)^2\left(-\frac{4}{315}\alpha^6+\frac{101}{4725}\alpha^8-\ldots\right)+\ldots. \quad (3.15)$$

In this model, α is the only parameter, which is scaled by $\sqrt{\epsilon}$ [as the transverse length $A'(x)$]. Indeed, after this scaling, the expansion (3.15) recovers the result of mapping (2.20) for $A'(x)=\alpha$, $\beta A(x)U'(x)=-\alpha\beta F x$, and all the higher derivatives of $A(x)$ and $U(x)$ being zero due to the linear boundary and the constant force.

The function $D(x)$ (3.13) is plotted in Fig. 1 for several values of α. It reduces to the formula (1.6) in the case of zero force. For F positive, its value rises to unit for any α. We can interpret this result within the picture mentioned when we analyzed $\rho_0(x,y)$ [Eq. (3.5)]. The particles fall in x direction under the constant force F with the mean velocity βF, but in y direction, they diffuse only to the distance $\sim\sqrt{x}$. For any $\alpha>0$, there exists a distance x, where the boundary $y=\alpha x$ is so far from the x axis that the particles cannot reach it by diffusion. Figure 2(a) shows the transverse profiles of $\rho(x,y)$

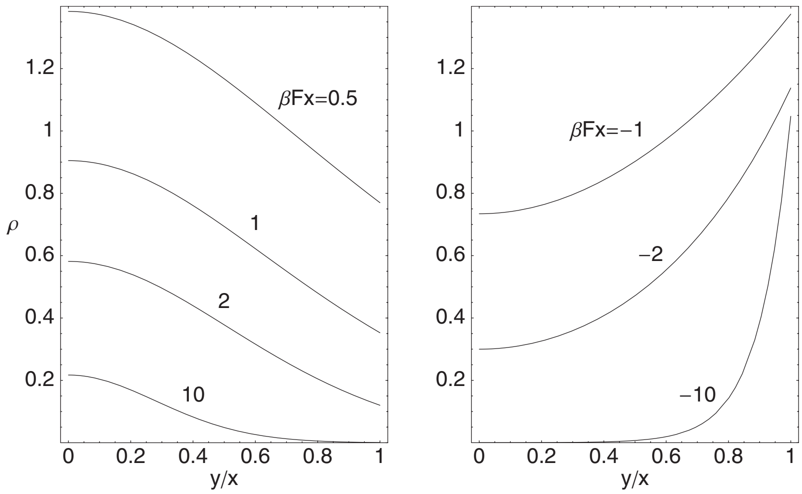

FIG. 2. Transverse profiles of the 2D density $\rho(x,y)$ in the cone bounded by $y=x$ for the force F positive (left) and negative (right picture).

generated by Eq. (3.11) for various βFx and $\alpha=1$, supporting this picture. Then $D(x)\to 1$ says that the boundary does not restrict the flowing particles for large βFx.

On the other hand, the case $F<0$ can be interpreted as a flow of particles falling from infinity into the cone and being absorbed when hitting the origin. As the force is not parallel to the slanted boundary, the particles are piled in its vicinity as it is shown in Fig. 2(b). The force obstructs the particles to diffuse to the origin, pushing them to the boundary, so the coefficient $D(x)$ is even lower than in the case of no force.

Finally, we discuss extensibility of the formula (1.6) for the forced diffusion. It is very difficult to sum directly some infinite group of terms in Eq. (2.20) to obtain an (approximate) formula for $D(x)$ in a concise form. The analysis for the diffusion alone [8] showed that the most effective way is to approximate the real boundary $y=A(x)$ at some x by the boundary of some exactly solvable model and to calculate $D(x)$ by taking the 2D stationary density for this model. For example, if the boundary of a real channel is replaced by the linear cone (Fig. 3), the formula (1.6) is obtained, hence, named the "linear approximation."

In this context, the exactly solvable model of the stationary diffusion in a homogeneous field can serve for finding an approximation of $D(x)$ for any boundary. The formula (3.13) reproduces exactly the expansion (2.20) up to the first derivatives of $U(x)$ and $A(x)$; i.e., it represents the exact sum of these terms. Neglecting A'' and the higher derivatives correspond again to replacing the real boundary $y=A(x)$ by its tangent, so we get an extended linear approximation. Without any calculation, the approximated $D(x)$ will be the formula (3.13) with the parameters α and βFx replaced by the local values of $A'(x)$ and $-\beta U'(x)A(x)/A'(x)$, respectively. For negative A', we use the symmetry of $D(x)$ seen in its expansion (3.15); the value of $D(x)$ is unchanged if the signs of both A' and $U'=-F$ are inverted.

We test this approximation on a periodic channel (Fig. 3) examined in Refs. [10–13]. We calculate the effective scaled mobility μ according to the modified Stratonovich formula

$$\mu(F)=\frac{\langle\dot{x}\rangle}{\beta F}=\frac{1-\exp(-\beta F)}{\beta F T_1(F)}, \qquad (3.16)$$

where the integral

$$T_1(F)=\int_0^1 dx\frac{e^{-\beta Fx}}{A(x)D(x)}\int_{x-1}^{x} dx' A(x')e^{\beta Fx'} \qquad (3.17)$$

comes from the mean first time of passage through one period of the channel, corrected by the effective coefficient $D(x)$ by Burada *et al.* [11,12]. We use our notation and the period $L=1$.

The results for the channel of $A(x)=1.02-\cos 2\pi x$ are plotted in Fig. 4 and compared with the mobility obtained from the FJ equation $[D(x)=1]$ and the linear approximation without field (1.6). Let us recall that the Brownian dynamic simulations (Fig. 2 in Ref. [12]) exhibit very good agreement with Eq. (1.5) for small forces, but with growing F, μ approaches 1 as predicted by the FJ approximation.

The linear approximation for nonzero forces based on the formula (3.13) (the dotted line) fails to improve the result of the standard linear approximation (1.6). Nevertheless, it is worth to analyze this failure. We refer to the stationary density in this channel as reported in Ref. [11] and presented in Fig. 5 there. The Brownian simulations showed that the particles diffuse as a narrow stream across the broad parts of the channel in strong fields. The particles are dragged by the force so fast that they have no time to diffuse in the transverse direction(s) and to explore the whole volume of the bulge. This is the same situation as we found for large βFx; the particles were not able to reach the boundary and the corresponding $D(x)$ approached unit. So we suppose that

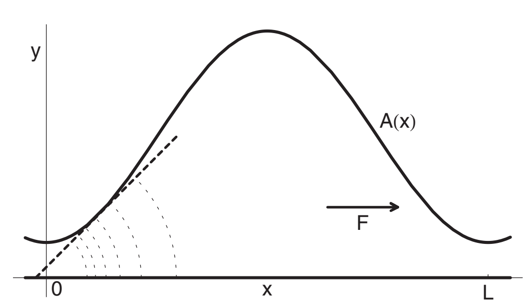

FIG. 3. Linear approximation: the boundary $y=A(x)$ is replaced by its tangent (thick dashed line) at some x and the exact 2D density is replaced by the density in the cone geometry (depicted by the dashed arcs).

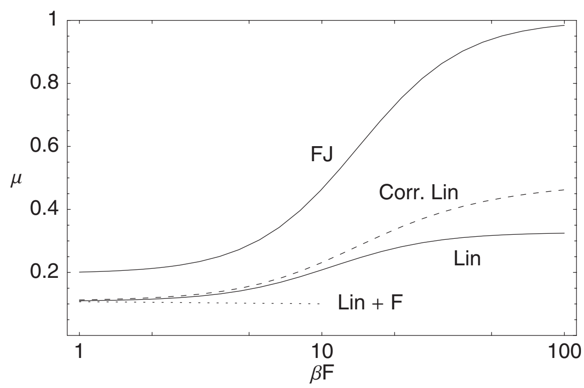

FIG. 4. The scaled mobility μ in the periodic channel with $A(x)=1.02-\cos 2\pi x$ depending on the applied force. The results are obtained from the FJ equation (FJ), the linear approximation (1.6) (Lin), the linear approximation extended for nonzero forces according to Eq. (3.13) (dotted line), and the linear approximation corrected only for positive FA' (dashed line).

$D(x)$ based on Eq. (3.13) approximates well the expanding part of the channel $x \in (0, L/2)$.

For $x > L/2$, $A'(x)$ becomes negative and the $D(x)$ according to Eq. (3.13) falls below the zero-force value (1.6). These values of the approximated $D(x)$ are calculated for an infinite cone, collecting the particles falling from infinity, so the particles are distributed mainly near the slanted boundary [see Fig. 2(b)]. The situation in the periodic channel is different; the particles not feeling the boundary continue to move in the stream near the x axis. So our approximation fails in this region and gives too big contributions to $T_1(F)$. If we do an *ad hoc* correction of $D(x)$ (for testing purposes) and take the zero-force formula (1.6) for negative FA', otherwise $D(x)$ according to Eq. (3.13), we obtain the dashed line in Fig. 4, which already improves the liner approximation.

Within the argumentation presented, $D(x)$ should be nearly unit until the particles start to hit the narrowing boundaries in front of the bottleneck at $x=L$. $D(x)$ should fall below the value of Eq. (1.6) here. After passing the bottleneck, $D(x)$ should rise again according to Eq. (3.13) and approach unit when the stream not feeling the boundaries is formed. Thus, only the region near the bottleneck gives $D(x) < 1$ in strong fields. It is getting smaller with growing force and so the mobility approaches the values predicted by the FJ equation.

Unfortunately, the extended linear approximation is not able to fulfill this scenario in a rigorous way (if we refuse to do some *ad hoc* modifications). Looking for better approximations, including probably higher derivatives of $A(x)$, is the task for the future.

IV. CONCLUSION

We showed in this paper that the diffusion in a channel of varying cross section $A(x)$ exposed to an external force parallel to the longitudinal direction can be mapped onto the longitudinal dimension in the same way as the diffusion alone. Instead of the diffusion equation, we start from the 2D (or more dimensional) Smoluchowski equation (2.1), where the anisotropy of the diffusion constant, equivalent to the scaling of the transverse lengths, can be introduced as well. This is used in the mapping procedure to project out the transients and to arrive rigorously at a 1D evolution equation of the Fick-Jacobs type (1.7).

In the case of instant equilibration in the transverse directions (infinite transverse diffusion constant), the mapped 1D equation is consistent with the concept of the "entropic potential;" the function $U_{ent}(x)=-k_B T \ln A(x)$ can be simple added to the real potential $U(x)$. This is not valid if the transverse relaxation is slower. The flux has to be corrected by an operator (2.10) in general, which becomes a function $D(x)$ in the limit of the stationary flow, an equivalent of the effective diffusion coefficient. In this case, it does not depend only on derivatives of $A(x)$ but also on derivatives of the potential $U(x)$. The expansion of $D(x)$ in the parameter of anisotropy ϵ (2.20) is generated by the mapping procedure up to an arbitrary order.

We tested this expansion on a model of the stationary diffusion in an infinite linear cone in a homogeneous field, which is exactly solvable. We found the exact formula for the corresponding coefficient $D(x)$. A simple analysis encourages us to interpret the resultant $D(x)$ as a coefficient reflecting how much the local shape of the boundary restricts the flow of the particles diffusing under the force. If the flow is not influenced by the boundary, $D(x) \to 1$, although the channel is not flat.

The formula for $D(x)$ in the cone (3.13) sums exactly all the terms in the expansion (2.20), depending only on $A'(x)$ and $U'(x)$. So it can be used for construction of the extended linear approximation, replacing the local boundary $A(x)$ by its tangent at a point x and considering the local force $F=-U'(x)$ to be constant. Although this strategy is successful for the diffusion alone [it yields the formulas (1.5) and (1.6), which are used in practice], its direct extension to the diffusion under a force has its limitations in strong fields. Presumably, the higher derivatives of $A(x)$ have to be included in an approximation working satisfactorily for typical shapes of the channels.

Nevertheless, the mapping showed in a rigorous way that correcting of the Fick-Jacobs equation by an effective coefficient $D(x)$ (1.7) is justified also in an external potential and looking for such a function is meaningful.

ACKNOWLEDGMENT

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APPENDIX: DETAILED CALCULATIONS

We give here detailed calculations connected with analysis of the stationary flow in the linear cone in a homogeneous potential and derivation of the corresponding formula for $D(x)$ [Eq. (3.13)].

The function $u(x,y)$, shaping the 2D density $\rho(x,y)$ according to Eq. (3.1), has the form (3.7) in the polar coordinates. If the analytic function $f(z)=g(z)\tanh(z/2)$ and

$g(t+i\phi)=g(t-i\phi)$, also the BC (3.8) at the boundary $y=\alpha x=(\tan\phi_0)x$ is satisfied.

Our first task is to calculate the flux J by direct calculation. We rewrite $u(r,\phi)$ by splitting Eq. (3.7) into two integrals, substituting for $z=t+i\phi$ and $z=t-i\phi$ in the relevant parts,

$$u(r,\phi)=\int_{i\phi}^{\infty+i\phi}e^{-(\beta Fr/2)\cosh(z-i\phi)}g(z)\tanh\frac{z}{2}dz + \int_{-i\phi}^{\infty-i\phi}e^{-(\beta Fr/2)\cosh(z+i\phi)}g(z)\tanh\frac{z}{2}dz, \quad (A1)$$

and by using $r\cosh(z\pm i\phi)=x\cosh z\pm iy\sinh z$ in the exponents, we restore the Cartesian coordinates. Next, we can change the integration paths

$$\int_{\pm i\phi}^{\infty\pm i\phi}\ldots dz \to \int_{\pm i\phi}^{0}\ldots dz+\int_0^{\infty}\ldots dz+\int_{\infty}^{\infty\pm i\phi}\ldots dz,$$

as the corresponding contours do not enclose any pole. The first integrals from both parts cancel one another and the last ones are zero. Finally,

$$\rho(x,y)=e^{\beta Fx/2}\int_0^{\infty}(e^{i(\beta Fy/2)\sinh z}+e^{-i(\beta Fy/2)\sinh z})e^{-(\beta Fx/2)\cosh z}g(z)\tanh(z/2)dz. \quad (A2)$$

We calculate the total flux

$$J=\int_0^{\alpha x}j_x(x,y)dy = -\int_0^{\alpha x}e^{\beta Fx}\partial_x[e^{-\beta Fx}\rho(x,y)]dy = -ie^{\beta Fx/2}\int_0^{\infty}(e^{i(\beta Fx\alpha/2)\sinh z}-e^{-i(\beta Fx\alpha/2)\sinh z})e^{-(\beta Fx/2)\cosh z}g(z)dz, \quad (A3)$$

after trivial integration over y. Now, we use the relation $\cosh z\pm i\alpha\sinh z=\cosh(z\pm i\phi_0)/\cos\phi_0$, split again the integral, and return the substitutions $t=z\pm i\phi_0$ in the relevant parts. Due to the BC, $g(t\pm i\phi_0)=\bar{g}(t)$ and both integrated functions are the same; we get

$$\left[\int_{-i\phi_0}^{\infty-i\phi_0}-\int_{i\phi_0}^{\infty+i\phi_0}\right]\exp\left(\frac{-\beta Fx\cosh t}{2\cos\phi_0}\right)\bar{g}(t)dt.$$

We can add the integral from $-i\phi_0$ to $i\phi_0$, which is zero due to symmetry, and close the loop in infinity, so

$$J=-ie^{\beta Fx/2}\oint\exp\left(\frac{-\beta Fx\cosh t}{2\cos\phi_0}\right)\bar{g}(t)dt, \quad (A4)$$

the integration contour is depicted in Fig. 5. For $g_0(z)=\coth(\pi z/2\phi_0)$, the function $\bar{g}_0(t)=\tanh(\pi t/2\phi_0)$ has poles at $t=\pm i\phi_0$, just in the corners of the contour. We replace this contour by three loops: the first one avoiding the poles and

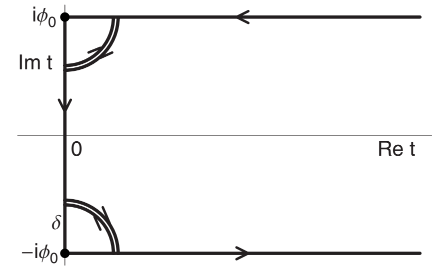

FIG. 5. Integration contour for the flux J.

two small sectors ($\delta\to 0$) in their vicinity. Integration around the first loop does not enclose poles, so it gives zero. The last ones are integrals of the type

$$\oint f(z)\frac{dz}{z}=\left[\int_{0^+}^{\delta}+\int_{\delta}^{i\delta}{}_{(arc)}+\int_{i\delta}^{i0^+}\right]f(z)\frac{dz}{z}\to i\frac{\pi}{2}f(0),$$

applying it on the integral (A4) for both poles, we arrive at $J=2\phi_0$ [Eq. (3.10)].

The other solutions generated by the functions $g(z)=\sinh(n\pi z/\phi_0)$ do not give rise to the poles of $\bar{g}(t)$ inside or at the contour (Fig. 5), so the corresponding 1D flux is zero; these modes are the transients.

Having calculated the 2D density $\rho(x,y)$ and the corresponding flux J, we can derive the effective coefficient $D(x)$ according to the formula (3.12). Nevertheless, the integration of $\rho(x,y)$ is difficult in our model, so we recast this relation into a form, in which only the 2D density at the slanted boundary $\rho_b(x)=\rho(x,\alpha x)$ is necessary.

First, we express the 1D density $p(x)$ by using $\rho_b(x)$ and J; the expression

$$e^{\beta Fx}\partial_x e^{-\beta Fx}p(x)=e^{\beta Fx}\partial_x\int_0^{\alpha x}e^{-\beta Fx}\rho(x,y)dy = e^{\beta Fx}\left\{\alpha e^{-\beta Fx}\rho(x,\alpha x)+\int_0^{\alpha x}\partial_x[e^{-\beta Fx}\rho(x,y)]dy\right\} = \alpha\rho_b(x)-J.$$

Hence, after integration over x,

$$p(x)=\frac{J}{\beta F}+\alpha e^{\beta Fx}\int e^{-\beta Fx}\rho_b(x)dx. \quad (A5)$$

Then from Eq. (2.17),

$$\frac{J}{D(x)}=-\alpha xe^{\beta Fx}\partial_x\left[\frac{1}{\alpha x}e^{-\beta Fx}p(x)\right] = J-\alpha\rho_b(x)+\frac{1}{x}\left[\frac{J}{\beta F}+\alpha e^{\beta Fx}\int e^{-\beta Fx}\rho_b(x)dx\right],$$

the most convenient form for our next purposes is obtained after integration by parts

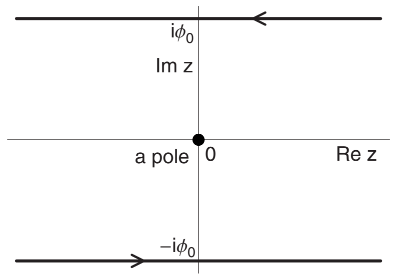

FIG. 6. Contour for the integral (A10).

$$\frac{1}{D(x)} = 1 + \frac{1}{\beta F x} - \frac{\alpha}{Jx} e^{\beta F x} \int x[e^{-\beta F x}\rho_b(x)]' dx. \quad \text{(A6)}$$

The integration constant has to be fixed to remove the divergent terms $\sim 1/\beta F x$.

Now, we express $[\exp(-\beta F x)\rho_b(x)]'$. Taking the formula (3.7) with $f(z)$ according to Eq. (3.11), we get

$$u(x,\alpha x) = \int_0^\infty \left[\tanh\frac{t+i\phi_0}{2} + \tanh\frac{t-i\phi_0}{2}\right] e^{-(\beta F r/2)\cosh t}\bar{g}(t)dt$$
$$= \int_0^\infty \frac{2\sinh t dt}{\cosh t + \cos\phi_0} e^{-(\beta F r/2)\cosh t}\tanh\frac{\pi t}{2\phi_0}, \quad \text{(A7)}$$

as $g(t\pm i\phi_0)=\bar{g}(t)=\tanh(\pi t/2\phi_0)$ at the boundary; $r=x/\cos\phi_0$. Then

$$[e^{-\beta F x}\rho_b(x)]' = [e^{-\beta F x/2}u(x,\alpha x)]'$$
$$= -\frac{2\pi}{\phi_0 x}e^{-\beta F x/2}\int_0^\infty e^{-(\beta F r/2)\cosh t}\frac{dt}{1+\cosh(\pi t/\phi_0)} \quad \text{(A8)}$$

after integrating by parts. Applying this relation in Eq. (A6), taking $J=2\phi_0$ and completing easy integration in x, we find

$$\frac{1}{D(x)} = 1 + \frac{1}{\beta F x} - \frac{2\pi\alpha}{\beta F x\phi_0^2}e^{\beta F x} \times\left\{\int_0^\infty \frac{dt}{(1+\cosh(\pi t/\phi_0))}\frac{\cos\phi_0}{(\cosh t+\cos\phi_0)} \times\exp\left[-\frac{\beta F x}{2}\left(\frac{\cosh t}{\cos\phi_0}+1\right)\right] + C_0\right\},$$

the integration constant C_0 is fixed to remove the diverging term proportional to $1/\beta F x$. As the integral

$$\int_0^\infty \frac{dt}{(1+\cosh\pi t/\phi_0)}\frac{\cos\phi_0}{(\cosh t+\cos\phi_0)} = \frac{\phi_0^2}{2\pi\alpha}, \quad \text{(A9)}$$

the constant $C_0=0$ and we arrive at the formula (3.13).

The integral (A9) and similar integrals obtained when $1/D(x)$ is expanded in $\beta F x$ are calculated by an integral

$$\oint iF(z)\frac{dz}{1-\cosh(\pi z/\phi_0)} \quad \text{(A10)}$$

along the contour in the complex plain depicted in Fig. 6. If we split it to the lower part and the upper part and substitute for the integration variable $z=t-i\phi_0$ and $z=t+i\phi_0$, respectively, we get

$$= i\int_{-\infty}^{\infty}[F(t-i\phi_0)-F(t+i\phi_0)]\frac{dt}{1+\cosh(\pi t/\phi_0)}.$$

The integral (A9) is related to Eq. (A10) for $F(z)=\tanh(z/2)$. Then the contour of Eq. (A10) encloses a simple pole at $z=0$. So we get

$$\frac{2\phi_0^2}{\pi} = \int_{-\infty}^{\infty}\frac{2\sin\phi_0}{(\cosh t+\cos\phi_0)}\frac{dt}{(1+\cosh\pi t/\phi_0)},$$

hence we obtain the relation (A9).

For any integral appearing in the expansion of $1/D(x)$ in $\beta F x$, one can find the corresponding function $F(z)$ and to express it explicitly. The most transparent way is to deal with a function

$$\Xi_a(\chi) = \int_0^\infty e^{-\chi\cosh t}\frac{adt}{1+\cosh(at)}, \quad \text{(A11)}$$

entering Eq. (A8), where $\chi=\beta F r/2$ and $a=\pi/\phi_0$. If it is (formally) expanded in χ, we get

$$\Xi_a(\chi) = \int_0^\infty \frac{adt}{1+\cosh(at)}\sum_{k=0}^{\infty}\frac{(-\chi)^k}{k!}\cosh^k t$$
$$= \int_0^\infty \frac{adt}{1+\cosh(at)}\left[I_0(-\chi)+2\sum_{n=1} I_n(-\chi)\cosh nt\right],$$

I_n are the Bessel functions. The function $F(z)=z$ in Eq. (A10) generates the coefficient at I_0 and $F(z)=\sinh nz$ is to be used to calculate the coefficients at I_n. The result

$$\Xi_a(\chi) = I_0(-\chi) + 2\sum_{n=1} I_n(-\chi)\frac{n\pi/a}{\sin(n\pi/a)} \quad \text{(A12)}$$

can be expanded in χ, applied in Eq. (A8), and integrated in Eq. (A6) to gain the expansion (3.14) of $1/D(x)$.

Let us notice that the coefficients at I_n for $n\geq a$ diverge; the function $\Xi_a(\chi)$ [and so $1/D(x)$ too] is not analytic at $\chi=0$ for any finite a. The summation in Eq. (A12) has the upper limit $a-1$ and there is a remainder $O(\chi^a)$ there. Still, we can use it for gaining the expansion (3.15) in χ and $\alpha=\tan\phi_0=\tan(\pi/a)$, i.e., for $1/a\to 0$, where all derivatives in χ exist.

Of course, the problem is to do an analytic continuation of the formula (3.13) for $F<0$ [or $\Xi_a(\chi)$ for $\chi<0$]. To resolve it, we return to the interpretation of the solutions of Eq. (3.2); the Bessel functions I_ν cannot be excluded in principle in confined geometries. Aside from K_ν, the solution $u(r,\phi)$ of Eq. (3.2) can contain also combinations of $I_\nu(-\beta F r)\cos n\phi$. To generalize it, we use the integral formula for I_ν [17],

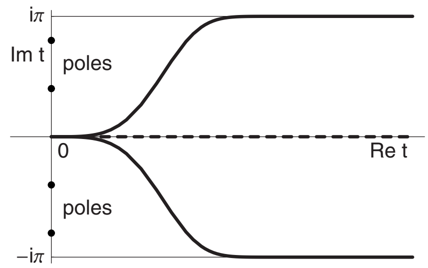

FIG. 7. Integration path for the negative forces (full line) and for the positive forces (dashed line).

$$I_\nu(r) = \frac{1}{\pi}\int_0^\pi e^{r\cos\theta}\cos\nu\theta d\theta - \frac{\sin\nu\pi}{\pi}\int_0^\infty e^{-\nu t - r\cosh t}dt$$
$$= \frac{1}{2\pi i}\left[\int_{-\infty-i\pi}^{-i\pi} + \int_{-i\pi}^{i\pi} + \int_{i\pi}^{\infty+i\pi}\right] e^{-\nu z - r\cosh z}dz,$$

if represented by an integral in the complex plain. This serves for our inspiration that the solution $u(r,\phi)$ (3.7) could be extended to negative forces F by changing the integration path from the positive part of the real axis to a line composed of $(0,\pm i\pi)$ and $(\pm i\pi, \infty \pm i\pi)$. We can check that the integral

$$\int_0^{\infty\pm i\pi} e^{(-\beta Fr/2)\cosh t}[f(t+i\phi)+f(t-i\phi)]dt \tag{A13}$$

solves Eq. (3.2) for negative F; if used in Eq. (3.2), the same condition $[f'(t+i\phi)+f'(t-i\phi)]|_{t=0}=0$ is obtained after double integration by parts. The treatment fixing the BC (3.8) remains the same, too, giving the condition $f(z) = g(z)\tanh(z/2)$ and $g(t+i\phi_0)=g(t-i\phi_0)$, which is to be satisfied for any (complex) t along the integration path.

The solution of our interest is generated again by $g(z) = \coth(\pi z/2\phi_0)$, but this function gives rise to poles on the imaginary axis. They have to be avoided from the right side, as depicted in Fig. 7. It becomes clear after calculation of the flux J, which is done in the same way as for $F>0$ [Eqs. (A1)–(A4)]. In the last step, the corresponding contour of the integral (A4) has to include only the poles at $t=\pm i\phi_0$ as in the case of positive force.

The final formula for ρ takes an average of the integrals over the upper and the lower paths for $F<0$ to provide a real value of the result. By construction, the integrals in Eq. (A8), $\Xi_a(\chi)$ [Eq. (A11)], and in $1/D(x)$ [Eq. (3.13)] have to be calculated in the same way, along the same path.

We can check the expansion of $\Xi_a(\chi)$ for $\chi<0$. The coefficients at $I_n(-\chi)$ are integrals of the same functions but are integrated along the changed path. Nevertheless, for $n<a$, the integrated functions are zero at $t\to\infty$ plus an arbitrary $i\phi$, so we can form a closed contour from the both paths, for the negative (full line) and the positive χ (the dashed line in Fig. 7). This contour does not enclose any pole of these functions, so the integration along both paths gives the same result. For any a, the first $a-1$ derivatives of $\Xi_a(\chi)$ at $\chi=0$ [as well as of $1/D(x)$ at $x=0$] are the same whether calculated for negative or positive χ; it can be considered as a "weak" analytic continuation of $\Xi_a(\chi)$ [Eq. (A11)] to negative χ.

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