Effective one-dimensional description of confined diffusion biased by a transverse gravitational force

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(Dated:)

Diffusion of point-like non interacting particles in a two-dimensional (2D) channel of varying cross section is considered. The particles are biased by a constant force in the transverse direction. We apply our recurrence mapping procedure, which enables us to derive an effective one-dimensional (1D) evolution equation, governing the 1D density of the particles in the channel. In the limit of stationary flow, we arrive at an extended Fick-Jacobs equation, corrected by an effective diffusion coefficient \( D(x) \), depending on the longitudinal coordinate \( x \). Our result is an approximate formula for \( D(x) \), involving also influence of the transverse force. Our calculations are verified on the stationary diffusion in a linear cone, which is exactly solvable.

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I. INTRODUCTION

A point-like particle diffusing in a two or three dimensional (2D,3D) channel of varying cross section became an archetypal model describing transport through nano channels, pores or along fibers in biological systems, as well as passing of large molecules through membranes. Analytic studies of such models usually require further simplifications, namely the dimensional reduction to a purely one-dimensional (1D) system described by an effective 1D evolution equation, governing the linear (1D) density \( p(x,t) \) depending on time \( t \) and the longitudinal coordinate \( x \). On the other hand, any simplification should retain all important features of the original full dimensional model. After the dimensional reduction, they are reflected in the structure of the effective equation.

The Fick-Jacob (FJ) equation \([1]\),

\[
\partial_t p(x,t) = D_0 \partial_x A(x) \partial_x \frac{p(x,t)}{A(x)},
\]

\( (1.1) \)
can serve as the simplest example of such an effective 1D equation for diffusion in a channel with reflecting walls; \( A(x) \) denotes the cross section area for 3D or the width for 2D channels at some \( x \), and \( D_0 \) is the diffusion constant. This equation maintains only the mass conservation along the channel with varying \( A(x) \). Introducing a spatially dependent effective diffusion coefficient \( D(x) \) in the effective equation \([2,3]\),

\[
\partial_t p(x,t) = \partial_x A(x) D(x) \partial_x \frac{p(x,t)}{A(x)},
\]

\( (1.2) \)
enables us also to respect boundary conditions (BC) and the local mass conservation at a point \((x,y)\) of the full dimensional problem in the case of the stationary flow, i.e. when the net flux \( J(x,t) \) flowing through the channel is constant \((y\) denotes the transverse coordinates). For nonstationary processes, one should replace the function \( D(x) \) by an operator \( \hat{D}(x) \), containing also the spatial derivatives \( \partial^n_x \), \( n = 1,2,... \), but in practice, in most cases the asymptotic behavior of the processes is studied and the FJ equation extended only by the function \( D(x) \), Eq. \( (1.2) \), represents a significant improvement of the standard FJ approximation \( (1.1) \).

Of course, it is necessary to find a way how to fix the function \( D(x) \). Based on a phenomenological argumentation, Reguera and Rubí \([4,5]\) suggested a function

\[
D(x) = D_0 \left[ 1 + h^2(x) \right]^{-\eta},
\]

\( (1.3) \)

where \( \eta = 1/3 \) or \( 1/2 \) for 2D or 3D channels with axial symmetry, respectively, and \( h(x) \) denotes half width or radius of the channel. Later Kalinay and Percus \([6,7]\) showed, that this function can be found as a series expansion in a small parameter \( \epsilon \), representing the ratio of the longitudinal and the transverse diffusion constant, \( \epsilon = D_0/D_y \). The anisotropy of the diffusion constant, imposed artificially, causes separation of the modes quickly decaying in the transverse direction from much slower longitudinal ones and formally, it enables us to find a recurrence scheme, generating systematically higher order corrections to the FJ equation \( (1.1) \), giving the expansion of the function \( D(x) \) in \( \epsilon \) in the stationary state. For 2D channels, bounded by \( y = h(x) \) and the \( x \) axis, we get

\[
D(x) = D_0 \left( 1 - \frac{\epsilon}{3} h'^2 + \frac{\epsilon^2}{45} h'' \times \left[ 9h'^3 + hh'' - h^3 h^{(5)} \right] - ... \right).
\]

\( (1.4) \)

If \( h''(x) \) and the higher derivatives are neglected, the result is

\[
D(x) \approx D_0 \left( 1 - \frac{\epsilon}{3} h'^2 + \frac{\epsilon^2}{5} h'^4 - ... \right) = D_0 \frac{\arctan \sqrt{h'}}{\sqrt{h'}},
\]

\( (1.5) \)
a function differing from \( (1.3) \) by less than 1% for moderate slopes, \( |h'| < 1 \), for an isotropic diffusion, \( \epsilon = 1 \). For 3D symmetric channels, the same treatment results in the formula \( (1.3) \) and \( \eta = 1/2 \). All formulas exhibited good agreement with numerical tests \([4,5] \) for \( |h'| < 1 \);
steeper slopes require to take also the higher derivatives of \( h(x) \) into account \([8]\), or to avoid the expansion for specific geometries at all \([9] - [13]\).

Let us remark that introducing anisotropy of the diffusion constant is equivalent to rescaling of all transverse lengths (i.e. the coordinate \( y \) and the half width \( h(x) \) in the 2D channels) by \( \sqrt{7} \) \([8]\). This scaling together with a similar recurrence procedure were used to calculate corrections to the mean velocity and the dispersivity of the particles \([14, 15]\) within the macrotransport theory, as well as for re-derivation of \( D(x) \) in Eq. \((1.5)\) \([16]\).

Recent studies \([17, 18]\) showed that the same strategy could be used also for the dimensional reduction of the Smoluchowski equation,

\[
\partial_t \rho(x, y, t) = \left[ D_0 \partial_x e^{-U(x,y)/k_B T} \partial_x e^{U(x,y)/k_B T} + \right. \\
D_y \nabla_y \cdot e^{-U(x,y)/k_B T} \nabla_y e^{U(x,y)/k_B T} \right] \rho(x, y, t), (1.6)
\]

i.e. for mapping of the diffusion in an external field \( U(x, y) \); \( \rho(x, y, t) \) is the 2D or 3D density, \( \nabla_y \) denotes the gradient in the transverse directions and \( T \) is the temperature. The ratio \( \epsilon = D_0/D_y \), remains a good small parameter also for the biased diffusion, enabling us again to construct a recurrence procedure generating systematically corrections to an equivalent of the FJ equation. This extension allows us to apply the dimensional reduction to a much broader class of problems interesting in chemical physics. Considering a force parallel to the \( x \) axis of the channel, we showed \([17]\) how the entropic potential is added to the real (energetic) one in the dimensionally reduced dynamics, which can be useful for studying e.g. the Brownian pumps \([19]\). Mapping of Eq. \((1.5)\) for a potential depending on the transverse coordinates \([18]\) can be used to get the reduced dynamics in a channel with soft walls.

In the present paper, we study diffusion in a 2D symmetric channel, bounded by smooth functions \( y = h(x) \) and \( -h(x) \), with hard and reflective walls (Fig.1). The particles are biased in the transverse direction by a constant gravitational force \( G \); the potential \( U(x, y) = G y \) in Eq. \((1.0)\). This model was investigated mainly in connection with the stochastic resonance during the last years \([20-24]\). An important feature of this model is an interplay between the gravitational force, holding particles in the potential wells in the wider parts of the channel, and the thermal motion, enabling the particles to diffuse into the neighboring compartments over the potential barriers formed by the narrowings of the channel. An oscillating force applied along the channel can help this hopping very effectively at a specific resonance frequency, depending on the force \( G \), the temperature \( T \) and the geometry of the channel.

We focus our attention on the competition between the gravitational potential and the "entropic" potential in diffusion through such channels. Our mapping procedure allows us to quantify their contributions to the net flow of particles in an elegant way: in the form of an effective 1D equation, involving both effects in its structure. The previous analyses used the 1D description, too, but governed by an equivalent of the FJ equation \((1.1)\). Comparison of this theory with the Brownian simulations \([25, 26]\) indicates that this approximation may be not satisfactory especially in the region of our interest, when both effects become comparable.

In the following section, we present the rigorous dimensional reduction of this model onto the longitudinal coordinate. We show how to merge the mapping of diffusion in a transverse field \([18]\) with the presence of the reflecting hard walls. The result of our mapping is an equation of the type \((1.2)\) in the limit of the stationary flow, with \( D(x) \) expanded to the first few orders in \( \epsilon \). In Section III, we suggest and justify an interpolation formula for \( D(x) \) based on results of the mapping procedure in the "linear approximation", when \( h/e(x) \) and higher derivatives in the expansion of \( D(x) \) are neglected. Our formula is verified by an exactly solvable model, the stationary diffusion of particles in a linear cone.

II. MAPPING PROCEDURE

We follow the procedure developed for the diffusion \([4, 6]\) and the biased diffusion \([17, 18]\), based on introducing a small parameter \( \epsilon \) into the 2D Smoluchowski equation \((1.0)\). We define it as a parameter of anisotropy of the diffusion constant, \( D_y = D_0/\epsilon \), but it can be also imposed by scaling of the transverse lengths \([16]\), \( y \to \sqrt{\epsilon} y \) and the inverse scaling of the force \( G \to G/\sqrt{\epsilon} \). Anyway, we get the equation

\[
\partial_t \rho(x, y, t) = \partial_x^2 \rho(x, y, t) + \frac{1}{\epsilon} \partial_y e^{-gy} \partial_y e^{gy} \rho(x, y, t) \quad (2.1)
\]

from Eq. \((1.0)\) for the model of our interest; we rescaled time \( t \) by the diffusion constant \( D_0 \), \( D_0 t \to t \), and \( g = G/k_B T \).

![FIG. 1: A sketch of the considered model: the channel is bounded by hard walls at \( y = h(x) \) and \( -h(x) \). Diffusing particles are biased by a constant gravitational force \( G \).](image)
The small parameter $\epsilon$ enables us to carry out two important steps of the mapping procedure. First, we can find readily the equivalent of the FJ equation in the limit $\epsilon \to 0$, and second, it becomes a parameter controlling the perturbation expansion of any quantity describing diffusion in the channel: the 2D density $\rho(x,y,t)$ and the flux density $j(x,y,t)$, or any mean value, like the mean velocity or dispersivity representing the mass conservation law, so the components of the flux density $j$ are

\[
\begin{align*}
    j_x(x,y,t) &= -\partial_x \rho(x,y,t), \\
    j_y(x,y,t) &= -\frac{1}{\epsilon} e^{-gy} \partial_y e^{gy} \rho(x,y,t).
\end{align*}
\] (2.2)

No flux through the reflecting hard walls requires to have the vector $j$ at the boundaries parallel to them, so we get

\[
e^{gy} \partial_y e^{-gy} \rho(x,y,t) = \pm \epsilon h'(x) \partial_x \rho(x,y,t) \bigg|_{y=\pm h(x)}
\] (2.3)

at the upper and the lower boundary $y = \pm h(x)$. BC at the ends of the channel are arbitrary, they do not enter the mapping procedure in our formulation. We can consider the channel as infinite.

The mapping procedure reduces the 2D Smoluchowski equation (2.1) governing the 2D density $\rho(x,y,t)$ to some 1D equation governing the 1D density $p(x,t)$, defined as

\[
p(x,t) = \int_{-h(x)}^{h(x)} \rho(x,y,t)dy.
\] (2.4)

Thus the first step of the mapping is integration of Eq. (2.1) over the cross section. Applying the definition (2.4) on the left hand side, we arrive at

\[
\partial_t p(x,t) = \int_{-h(x)}^{h(x)} \partial_x^2 p(x,y,t)dy - \frac{1}{\epsilon} \int_{-h(x)}^{h(x)} \left[ e^{-gy} \partial_y e^{gy} \rho(x,y,t) \right] dy
\] (2.5)

after integrating by parts and using BC (2.3).

Our goal is also to express the right hand side of Eq. (2.5) in terms of $p(x,t)$ instead of $\rho(x,y,t)$. This task is easy to complete in the limit $\epsilon \to 0$. For an infinitesimally small $\epsilon$, the transverse diffusion constant $D_y$ becomes almost infinite and the 2D density $\rho$ is equilibrated in the transverse direction almost immediately after any change in the $x$ direction. So we can write

\[
\rho_0(x,y,t) = \frac{1}{A(x)} e^{-gy} p(x,y),
\] (2.6)

where $A(x)$ provides normalization of $\rho_0$. If substituted in the condition (2.3), we have to obtain an identity. Hence

\[
A(x) = \int_{-h(x)}^{h(x)} e^{-gy} dy = \frac{2}{g} \sinh [gh(x)].
\] (2.7)

If we use the formula (2.6) for the 2D density in Eq. (2.5), we find

\[
\partial_t p(x,t) = \partial_x \int_{-h(x)}^{h(x)} e^{-gy} dy \cdot \partial_x \frac{p(x,t)}{A(x)} = \partial_x A(x) \partial_x \frac{p(x,t)}{A(x)},
\] (2.8)

which is (an equivalent of) the FJ equation (1.1). Let us stress that $A(x)$ is not the width of the channel here, but the integral (2.7). On the other hand, for $g \to 0$, $A(x)$ becomes $2h(x)$.

For $\epsilon > 0$, the transverse diffusion constant $D_y$ is finite and the local equilibrium in the $y$ direction is disturbed by the flux flowing along the curved boundaries at a given $x$. So the formula (2.6) cannot be used for the 2D density $\rho_0(x,y,t)$ does not satisfy the Smoluchowski equation (2.1). The small parameter $\epsilon$ enables us to look for deviations of the real 2D density $\rho(x,y,t)$ from the equilibrated density $\rho_0$ (2.6) in the form of a sequence of corrections, as an expansion in powers of $\epsilon$.

Instead of expanding some specific density $\rho(x,y,t)$ in $\epsilon$, we prefer a more general method. We look for the expansion of a wide class of solutions of the 2D problem; we expand all $\rho(x,y,t)$, which can be generated from any 1D solution $p(x,t)$ of the searched 1D equation by the backward mapping onto the space of solutions of the 2D problem. Formally, these 2D densities can be expressed by the formula

\[
\rho(x,y,t) = e^{-gy} \hat{\omega}(x,y,\partial_x) \frac{p(x,t)}{A(x)},
\] (2.9)

where $\hat{\omega}$ represents an operator of the backward mapping. It acts on a wide class of $p(x,t)$, so the dependence of $p(x,t)$ on $\epsilon$ is not important, we take it as an unfixed function. Instead, we look for expansion of the operator $\hat{\omega}$ in $\epsilon$, so

\[
\rho(x,y,t) = e^{-gy} \sum_{n=0}^{\infty} \epsilon^n \hat{\omega}_n(x,y,\partial_x) \frac{p(x,t)}{A(x)}.
\] (2.10)

We know already the zero-th order term, $\hat{\omega}_0 = 1$, which gives the equilibrated solutions $\rho_0$ (2.6) in the limit $\epsilon \to 0$.

Supposing $\rho(x,y,t)$ of the form (2.10), we can formally complete the construction of the 1D evolution equation. Applying this expression in Eq. (2.5), we find

\[
\partial_t p(x,t) = \partial_x \int_{-h(x)}^{h(x)} dy e^{-gy} \partial_x \sum_{n=0}^{\infty} \epsilon^n \hat{\omega}_n(x,y,\partial_x) \frac{p(x,t)}{A(x)}.
\]
Here we already applied \( \dot{\omega}_0 = 1 \) and introduced an operator \( \dot{Z} \), correcting the FJ equation \((2.8)\). It can also be expanded in \( \epsilon \),

\[
\epsilon \dot{Z}(y, \partial_x) = \sum_{k=1}^{\infty} \epsilon^k \dot{Z}_k(y, \partial_x); \\
\dot{Z}_k(y, \partial_x) = -\frac{1}{A(x)} \int_{-h(x)}^{h(x)} dy e^{-gy} \dot{\omega}_k(y, x, \partial_x). \tag{2.12}
\]

Finally, the 2D density \((2.10)\) has to be a solution of the original Smoluchowski equation \((2.1)\),

\[
\int_{-h(x)}^{h(x)} dy e^{-gy} \dot{\omega}_n(y, x, \partial_x) = 0, \tag{2.13}
\]

which generates a recurrence relation fixing the operators \( \dot{\omega}_n \). Because we suppose that these operators act only on the spatial coordinates, the time derivative commutes with them and for \( \partial \partial_x p(x, t) \), we use the equation \((2.11)\). Collecting the terms at the same powers of \( \epsilon \), we find

\[
\partial_y e^{-gy} \partial_y \dot{\omega}_{n+1}(y, x, \partial_x) = -e^{-gy} \left[ \partial_x^2 \dot{\omega}_n(y, x, \partial_x) + \sum_{k=0}^{n} \dot{\omega}_{n-k}(y, x, \partial_x) \frac{1}{A(x)} \partial_x A(x) \dot{Z}_k(y, x, \partial_x) \partial_x \right]. \tag{2.14}
\]

we take \( \dot{Z}_0(y, x, \partial_x) = -1 \) in this formula. After double integration, we obtain \( \dot{\omega}_{n+1} \), giving the \( n+1 \)-st correction to the 2D density, if applied on some 1D solution \( p(x, t) \).

Two integration constants have to be fixed (they are also operators, but independent of \( y \)). The first one provides satisfaction of the BC \((2.3)\). Using the formula \((2.10)\) in Eq. \((2.3)\) and comparing the terms at the same powers of \( \epsilon \), we get the condition

\[
\partial_y \dot{\omega}_{n+1}(y, x, \partial_x) = \pm h'(y) \partial_x \dot{\omega}_n(y, x, \partial_x) \bigg|_{y=\pm h(x)}. \tag{2.15}
\]

If the integration constant is fixed at one boundary, the BC at the opposite boundary is automatically satisfied. The second integration constant helps to satisfy the normalization condition; applying the formula \((2.10)\) in the definition \((2.4)\) has to give identity in any order of \( \epsilon \), hence

\[
\int_{-h(x)}^{h(x)} dy e^{-gy} \dot{\omega}_n(y, x, \partial_x) = 0 \tag{2.16}
\]

calculated according to the formula \((2.12)\). Calculation of the first order correction and other details are given in the Appendix A. We show here only the results,

\[
\dot{\omega}_1 = \frac{h'}{g} \left[ e^{gy} + (1 - gy) \cosh gh - gh \left( \frac{1}{\sinh gh} + 2 \sinh^2 \frac{gh}{2} \right) \right] \partial_x \tag{2.17}
\]

and the corresponding

\[
\dot{Z}_1 = \frac{h^2}{2 \sinh^2 gh} \left[ 1 + \cosh 2gh - 2gh \coth gh \right]. \tag{2.18}
\]

One can check that in the limit \( g \to 0 \), we obtain \( \dot{Z}_1 \to h^2/3 \), known for the diffusion alone \([2, 3]\). The higher order operators \( \dot{Z}_n \) starting from \( n = 2 \) also contain the spatial derivatives \( \partial_x \), what makes the equation \((2.11)\) too difficult for direct use in practice. Alike the diffusion alone \([3]\), this equation can be simplified by replacing the correction operator \( -\epsilon \dot{Z} \) by the function \( D(x) \) in the limit of the stationary state, when the net flux changes very slowly.

In that case, Eq. \((2.11)\) is replaced by an equation of the form \((1.2)\), where \( A(x) \) is given by the formula \((2.7)\) and \( D(x) \) has to be fixed. Thus we have two different expressions for the net flux,

\[
J(x, t) = -A(x) \left[ 1 - \epsilon \dot{Z}(x, \partial_x) \right] \partial_x \frac{p(x, t)}{A(x)} \tag{2.19}
\]

and

\[
J(x, t) = -A(x) D(x) \partial_x \frac{p(x, t)}{A(x)}, \tag{2.20}
\]

coming from Eqs. \((2.11)\) and \((1.2)\), respectively, as both equations represent the 1D mass conservation law. In the stationary state, \( J(x, t) = J \) is constant in time and space and \( \partial_x [p(x, t)/A(x)]/J = -1/A(x) D(x) \) depends only on geometry and the parameters of the model for any stationary solution \( p(x, t) = p(x) \). Then the formula \((2.19)\) describes the same flux \( J \) only if

\[
\frac{1}{D(x)} = A(x) \left[ 1 - \epsilon \dot{Z}(x, \partial_x) \right]^{-1} \frac{1}{A(x)}, \tag{2.21}
\]

which fixes the effective diffusion coefficient \( D(x) \) unambiguously for \( \dot{Z} \) obtained from the mapping procedure. If the expansion of \( \dot{Z} \) in \( \epsilon \) \((2.12)\) is used in Eq. \((2.21)\), the result is an \( \epsilon \)-expansion of \( D(x) \),

\[
D(x) = 1 - \frac{\epsilon h^2}{\sinh^2 gh} \left[ 1 + \cosh 2gh - 2gh \coth gh \right] \\
+ \frac{\epsilon^2 h^4}{\sinh^4 gh} \left[ \sinh^4 gh \cosh^2 gh - \frac{gh}{2} \sinh(2gh) \right] \\
x \left( 17 \sinh^2 gh + 36 \right) + (gh)^2 (7 \sinh^4 gh \right) \\
+ 40 \sinh^2 gh + 36 \right) + O(\epsilon^3) + O(h'''); \tag{2.22}
\]

the second and higher derivatives of \( h(x) \) are already neglected in this formula.
we recover correctly the first order term of $D(x)$ in Eq. (2.22). Then in strong fields, the formula (3.2) approaches the exact limit (3.1) and for $g \to 0$, we get the function of Reguera and Rubí, Eq. (1.3).

We compare first our interpolation formula with the true expansion of $D(x)$ (2.22) calculated up to the 4-th order in $\epsilon$. The plots of $D(x)$ versus role of the boundaries $h'(x)$ are depicted in Fig. 2. The thick lines describe the limits, $g \to 0$ and $\infty$. The dashed lines plot the formula (3.2) for three intermediate values of $g = 0.5, 1$ and $2$. These data are compared with the truncated series (2.22), the adjacent thin lines include the corrections up to the 3-rd order (the lower lines), and the 4-th order (the upper lines). In the region of fast convergence of the series (2.22), where the lines of the 3-rd and the 4-th order formulas almost coincide, the difference between the true and the interpolated values is comparable with the difference between the formulas (1.3) and (3.1) (the thick dashed line).

Unfortunately, the radius of convergence of this series is finite and decreasing with growing $g$. So we test our interpolation formula on an exactly solvable model.

Tests of such theories are often based on calculation of the net flux $J$ flowing through an exactly solvable structure. The flux calculated from the exact 2D density $\rho(x,y)$,

$$J = \int_{-b(x)}^{b(x)} j_x(x,y)dy = -\int_{-b(x)}^{b(x)} \partial_x \rho(x,y)dy \quad (3.4)$$

in the stationary regime, is compared with the corresponding flux according to Eq. (2.20) with $D(x)$ derived within the tested theory. We modify this method: for a given exact solution $\rho(x,y)$, we calculate the flux $J (3.4)$, the 1D density $p(x)$ (2.4) and the corresponding $D(x)$,

$$D(x) = -\frac{J}{A(x)} \left(\partial_x p(x)/A(x)\right)^{-1} \quad (3.5)$$

from Eq. (2.20), which is compared with $D(x)$ coming from the theory, Eq. (3.2) or (2.22) in our case.

Our exactly solvable model is a stationary flow through a linear cone, bounded by $y = \pm \alpha x$, see Fig. 3. The

FIG. 2: The coefficient $D(x)$ depending on the local slope $h'(x)$ and the values of $gh(x) = 0, 0.5, 1, 2$ and infinity at some point $x$. The thick lines depict the limits $g \to 0$ and $\infty$. The dashed lines correspond to the interpolation formula (3.2) with the exponent $-\eta$. The adjacent thin full lines describe the truncated expansion (2.22) up to the 3-rd order (the lower lines) and the 4-th order (the upper lines). The dots depict the data gained from the exactly solvable model, a linear cone with $h'(x) = \tan(\pi/10) \approx 0.325$ and $\tan(\pi/6) = 1/\sqrt{3}$.

FIG. 3: Linear cone with a constant transverse force $G$. The slopes of the walls, $h'$, corresponds to the unbiased diffusion, the coefficients limits: for $h' \to 0$, $D \to D_0 [1 + h'^2]^{\eta}$ with the exponent $-\eta$ depending on $gh(x)$, the proof is given in the Appendix A.

Finally, we recall that the formula (1.3) differs only slightly from the exact result, Eq. (1.5), at moderate slopes of the walls, $|h'(x)| < 1$. Then it seems reasonable to suggest this formula also for the region of intermediate $g$, but with the exponent $-\eta$ depending on $gh(x)$,

$$D(x) \approx D_0 [1 + h'^2(x)]^{-\eta[gh(x)]} \quad (3.2)$$

For the choice

$$\eta[gh(x)] = \frac{1}{\sinh^2 gh} [1 + \cosh^2 gh - 2gh \coth gh] \quad (3.3)$$

we recover correctly the first order term of $D(x)$ in Eq. (2.22). Then in strong fields, the formula (3.2) approaches the exact limit (3.1) and for $g \to 0$, we get the function of Reguera and Rubí, Eq. (1.3).

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in the stationary regime, is compared with the corresponding flux according to Eq. (2.20) with $D(x)$ derived within the tested theory. We modify this method: for a given exact solution $\rho(x,y)$, we calculate the flux $J (3.4)$, the 1D density $p(x)$ (2.4) and the corresponding $D(x)$,

$$D(x) = -\frac{J}{A(x)} \left(\partial_x p(x)/A(x)\right)^{-1} \quad (3.5)$$

from Eq. (2.20), which is compared with $D(x)$ coming from the theory, Eq. (3.2) or (2.22) in our case.

Our exactly solvable model is a stationary flow through a linear cone, bounded by $y = \pm \alpha x$, see Fig. 3. The
particles are emitted from a point-like source at the origin of the coordinate system and collected at an absorbing boundary placed far from the positions $x$ of our interest. Let us notice that the expansion (2.22) of $D(x)$ summed up to infinity describes our model exactly; $h'(x) = \alpha$ is constant and its derivatives are zero.

In the Appendix B, we show that the 2D density expressed in the form of an integral in the complex plane

$$
\rho(x, y) = e^{-gy/2} \int_0^\infty e^{-(g\sqrt{x^2+y^2}/2)\cosh(z-i\pi/2)} dz + c.c., (3.6)
$$

$\phi = \arctan y/x$ and $f(w) = \coth(mw/2)\tanh(w/2)$, $m = 3, 5, 7, ...$, represents a stationary solution of the Smoluchowski equation (2.21) with BC (2.3). $\epsilon = 1$, $D_0 = 1$ and $h(x) = \alpha x$ for specific values of the slope $\alpha = \tan\phi_0$; $\phi_0 = \pi/2m = \pi/6, \pi/10, ...$. The integration from 0 to $i\pi/2 + \infty$ (and to $-i\pi/2 + \infty$ in the complex conjugated expression) is carried out along any path avoiding the poles of the integrand on the imaginary axis from the right side, see Fig. 7 in the Appendix B. The contour plots of the density $\rho$ (3.6) and the corresponding $\bar{\rho}(x, y) = e^{3\pi/2}\rho(x, y)$ are shown in Fig. 4. According to Eq. (2.22), the gradient of $\bar{\rho}(x, y)$ is proportional to the flux density, so one can check visually on the right panel that the no flux BC are satisfied on both boundaries.

For testing the interpolation formula (3.2), we use the channels with $\alpha = \tan(\pi/6) = 1/\sqrt{3}$ and $\tan(\pi/10) \approx 0.325$. The values of $\rho(x)$ and $J$ in Eq. (3.6) were integrated numerically; the calculation of $J$ serves as a test of the numerical method, since $J$ does not depend on $x$. A choice of the force $g$ is not important; it scales the length unit in both directions, as can be seen from Eq. (3.6). Finally, we express $\alpha$ and $x$ by using $h(x)$ and $h'(x)$, $\alpha = h'(x)$ and $x = h(x)/h'(x)$, valid for the linear cone, to place the results in the plot of $D(x)$ depending on $h'(x)$ and $gh(x)$.

The data for $gh(x) = 0.5, 1$ and $2$ are depicted as dots in Fig. 2. The interpolation formula describes the coefficient $D(x)$ satisfactorily for small slopes of the boundaries $h'$ and close to the limits $gh(x) \to 0$ and $\infty$. For larger $h' > 0.5$ in an intermediate region, roughly $1 < gh(x) < 5$, the deviations are more notable. For practical purposes, one could try to find an interpolation formula for $\eta$ fitting better the exact data obtained for the linear cones. The exponents of Eq. (3.2) fitted to the exact values of $D(x)$ for the cones with $\alpha = \tan(\pi/6)$ (the larger dots) and $\tan(\pi/10)$ (the smaller dots) are depicted in Fig. 5 and compared with the function (3.3).

**IV. CONCLUSION**

The main aim of this paper was to arrive at an effective 1D description of diffusion in a 2D symmetric channel of varying width $2h(x)$. The diffusing particles are biased by a constant gravitational force $G$ acting in the direction perpendicular to the axis of the channel.

Our effective equation of the type (1.2), governing evolution of the 1D density $p(x, t)$ in the channel, goes beyond the Fick-Jacobs approximation, considering only instant equilibration of the 2D density in the transverse direction, which was used in the studies based on this model till now. The effects of slower transverse relaxation are included in the effective diffusion coefficient $D(x)$. We calculate this function within a recurrence procedure (3.1), mapping rigorously the 2D problem onto the longitudinal coordinate $x$ in the limit of the stationary flow, i.e. when the net flux changes very slowly with respect to the relaxation in the transverse direction.

The result is an expansion of $D(x)$ (2.22) in a parameter $\epsilon$ expressing the ratio of the diffusion constant in the longitudinal and the transverse directions, $\epsilon = D_0/D_0$, introduced artificially in the Smoluchowski equation (2.1) and set to 1 at the end. Adding the transverse force...
makes the result much more complicated, if compared with $D(x)$ (1.3) for the diffusion alone. It is difficult to obtain a simple formula usable in practice by direct summing of the expansion in $\epsilon h^2(x)$ up to infinity. So we suggest to use the interpolation formula (3.3) introduced before by Reguera and Ruh [3] for diffusion. We showed that the biasing force effectively changes the exponent $\eta$, depending on $gh(x)$, $g = G/k_B T$. It increases from $1/3$ for negligible $G$ up to $1$ in strong fields. This dependence can be approximated by the function (3.3); then the first order correction of the exact $D(x)$ (2.18) is recovered.

The interpolation formula is compared with the truncated exact expansion (2.22) up to the $4$-th order and also checked by the model of biased diffusion in a linear cone, which is exactly solvable. The agreement is satisfactory, checked by the model of biased diffusion in a linear cone, cated exact expansion $A$ and also

of the results.

Let us recall that the “linear approximation” does not can be approximated by the function (3.3); then the first

giving (A1).

After applying Eq. (2.7) and the first integration,

\[ \hat{\xi} = e^{g(\eta - h(x))} (1 + \coth g h(x)) \frac{d}{dx}. \]

(A3)

Notice that $\hat{\xi}$ is an operator, but independent of $y$. Also one can check that the relation

\[ \hat{\xi} = e^{g(\eta - h(x))} \left[ 1 + \coth g h(x) \right] \frac{d}{dx}. \]

(A5)

and fixing the second integration constant $\hat{\xi}$ (again an operator) from the normalization condition (2.10). After some algebra, we arrive at the formula (2.17). Finally, applying Eq. (2.16) to the resultant $\hat{\xi}$ gives the first order correction operator $\hat{\xi}$ (2.18).

In the limit $g \to \infty$, we keep only the leading terms of any expression during the calculation; the other terms, proportional to powers of $e^{-gh(x)}$ are negligible. For $A(x) \approx (1/g)e^{gh(x)}$, the initial equation (A1) of the recurrence scheme becomes

\[ \hat{\xi} = \frac{h(x)}{\sinh gh(x)} \left[ e^{gh} - \cosh gh(x) \right] \frac{d}{dx}. \]

(A4)

satisfies the BC (2.15) at the lower boundary, $y = -h(x)$, too. The next step is integration of Eq. (A3),

\[ \hat{\xi} = h(x)e^{-gh(x)} \left[ 1 + \coth gh(x) \right] \frac{d}{dx}. \]

(A3)

\[ \hat{\xi} = h(x) \left( 2e^{g(y - h(x))} - 1 \right) \frac{d}{dx}. \]

(A7)

BC are satisfied at the lower boundary, too, because the term $\sim e^{-2gh(x)}$ is negligible. The second integration and fixing the normalization condition gives

\[ \hat{\xi} = h(x) \left[ 2e^{g(y - h(x))} - y + \frac{1}{g} \coth g h(x) \right] \frac{d}{dx}. \]

(A8)

up to the terms $\sim e^{-gh(x)}$ and smaller. Finally, in the integration of $\hat{\xi}_1$ according to Eq. (2.12), only one term remains,

\[ \hat{\xi}_1 = ge^{gh(x)} \int_{-h(x)}^{h(x)} dy e^{-gh} h^2(x) \simeq h^2, \]

(A9)

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APPENDIX A: DETAILS OF MAPPING

We demonstrate here the mapping procedure on calculation of the first order correction and then we prove the formula (3.1) in the limit of large $g$.

Starting from the zero-th order, we take $n = 0$ in the recurrence relation (2.14), $\hat{\xi}_0 = 1$ and $\hat{\xi}_0 = -1$. We obtain

\[ \hat{\xi} = e^{-gh} \frac{d}{dx} = e^{-gh} \left( \frac{1}{A} \frac{d}{dx} A - \frac{d}{dx} A^2 \right) = e^{-gh} A' \frac{d}{dx}. \]
nonexponential in the limit of large $g$. Notice also that the exponential term in Eqs. (A7) and (A8) does not contribute to $C_0$ and $Z_1$; we can neglect it. This simplification corresponds to fixing $C_1$ at the lower boundary, then $\partial_y \omega_1 = -h'(x)\partial_x$. The BC at the upper boundary is not satisfied, but on the other hand, there are no particles there for large $g$, we treat the upper boundary like it was in infinity.

Now we can prove the formula (3.1). First we simplify the equation (2.21),

$$\frac{1}{D(x)} = A(x) \left[ 1 + \epsilon \hat{Z} + \epsilon^2 \hat{Z}^2 + \ldots \right] \frac{1}{A(x)} \approx 1 - \epsilon A(x) \hat{Z} \frac{1}{A(x)} + \left[ \epsilon A(x) \hat{Z} \frac{1}{A(x)} \right]^2 + \ldots$$  \hspace{1cm} (A10)

hence

$$D(x) \approx 1 - \epsilon A(x) \hat{Z} \frac{1}{A(x)} = 1 - \sum_{n=1}^{\infty} e^n A(x) \hat{Z}_n \frac{1}{A(x)};$$  \hspace{1cm} (A11)

the difference depends on derivatives higher than $h'(x)$ and they are neglected in our “linear” approximation.

The terms of the series in Eq. (A11) can be expressed directly by applying the operators $\hat{\omega}_n$ on a function $f(x) = \int dx / A(x) \approx \int ge^{-gh(x)}dx$. Then

$$A(x) \hat{Z}_n \frac{1}{A(x)} = -\int_{-h(x)}^{h(x)} dy e^{-gy} \partial_y \hat{\omega}_n f(x)$$  \hspace{1cm} (A12)

from the relation (2.22). The functions $\hat{\omega}_n f(x)$ are derived by the same recurrence procedure, as it was demonstrated on the operator $\hat{\omega}_1$ above. If we retain only the leading terms in the limit $g \to \infty$ in our expressions and neglect $h''(x)$ and its derivatives, we arrive at

$$\hat{\omega}_1 f(x) = -h'(x)e^{-gh(x)} \left[ g(y + h(x)) + 1 \right],$$

$$\hat{\omega}_2 f(x) = -\frac{h^3}{2} e^{-gh} \left[ g^2(y + h)^2 - 4g(y + h) + 2 \right],$$

$$\hat{\omega}_3 f(x) = -\frac{h^6}{6} e^{-gh} \left[ g^3(y + h)^3 - 9g^2(y + h)^2 + 18g(y + h) - 6 \right],$$

$$\hat{\omega}_n f(x) = -h'^{2n-1} e^{-gh} \sum_{k=0}^{n} \frac{(-1)^{n-k}}{k!} \frac{n!}{k!} \left[ g(y + h) \right]^k.$$  \hspace{1cm} (A13)

We can check normalization (2.16) of these formulas,

$$\int_{-h}^{h} dy e^{-gy} \sum_{k=0}^{n} \frac{(-1)^{n-k}}{k!} \frac{n!}{k!} \left[ g(y + h) \right]^k \approx \sum_{k=0}^{n} \frac{(-1)^{n-k}}{g} \frac{n!}{k!} \int_{0}^{\infty} e^{-z \cdot k}dz = 0, \hspace{1cm} (A14)$$

after substituting $z = g(y + h)$ and replacing the upper boundary $2gh$ by infinity; we omitted writing explicit dependence of $h(x)$ on $x$. The coefficients of the expansion (A11) are integrated in a similar way; after completing the $x$ derivative of the formulas (A13) in Eq. (A12) and using the normalization (A14), only the term

$$A(x) \hat{Z}_n \frac{1}{A(x)} = \int_{-h}^{h} gdye^{-gy}h^{2n} \sum_{k=1}^{n} \frac{(-1)^{n-k}}{(k-1)!} \frac{n!}{k!} \left[ g(y + h) \right]^{k-1} = h'^{2n} \sum_{k=1}^{n} \frac{(-1)^{n-k}}{k!} = -(1)^{n+1}h'^{2n}$$  \hspace{1cm} (A15)

remains, the result we wanted to prove.

Finally, one can check by direct calculation that the formulas (A13) satisfy the recurrence relation (2.14) and the BC (2.15) at the lower boundary. The operators $\hat{\omega}_n$ are replaced here by the functions $\hat{\omega}_n f(x)$, $\partial_y \hat{\omega}_n f(x) = ge^{-gh(x)}$. The terms depending on $\hat{Z}_k$ disappear from Eq. (2.14), since $A(x) \hat{Z}_n (1/A(x)) = -(1)^{n+1}h'^{2n}$ according to Eq. (A15), and its derivative depends on $h''$, which is neglected.

**APPENDIX B: EXACT SOLUTION**

We present here the stationary solution of the Smoluchowski equation (2.21) for the biased diffusion in a linear cone.

For a point-like source of particles placed at the origin of the coordinate system, the stationary equation (2.21),

$$0 = \partial_x^2 \rho(x, y) + \partial_y e^{-gy} \partial_x e^{gy} \rho(x, y)$$  \hspace{1cm} (B1)

becomes separable after substitution

$$\rho(x, y) = e^{-gy/2} u(x, y)$$  \hspace{1cm} (B2)

and converting to the polar coordinates, $x = r \cos \phi$, $y = r \sin \phi$,

$$\frac{1}{r} \partial_r r \partial_r + \frac{1}{r^2} \partial_\phi^2 \left( \frac{g}{2} \right)^2 u(r, \phi) = 0. \hspace{1cm} (B3)$$

The particular solutions are $u(r, \phi) = R_n(r/gr/2)e^{in\phi}$; $R_n$ stands for the Bessel $I_n$ or the Bessel $K_n$ functions. In an unbounded plane, the linear combinations describing the biased diffusion cannot contain the $I_n$ functions, since $\rho(x, y)$ would diverge for $y \to -\infty$. The solution $u(x, y)$ is then composed from the Bessel $K_n$ functions. The “ground-state” solution $u_0(r, \phi) = K_0(gr/2)$ carries the flux along the force. Other particular solutions $u_n(r, \phi) = K_n(gr/2) \sin(n\phi)$ are necessary for fitting $\rho(x, y) = 0$ at an absorbing boundary, if it is considered, but they do not contribute to the net flux; one can check that

$$\int_{-\infty}^{\infty} e^{-gy} \partial_y \left[ u_n(x, y)e^{gy/2} \right] dx = -J\delta_{n,0} \hspace{1cm} (B4)$$
at any fixed $y < 0$ (below the source). We need only the ground state $u_0(x, y)$ for the calculation of $D(x)$, Eq. [4.5].

Our problem is to find such a solution for diffusion in a linear cone, i.e. satisfying the BC (2.3) at $y = \pm \alpha x$. In the polar coordinates, the BC become

$$\partial_\phi u(r, \phi) = -\frac{gr}{2} \cos(\phi)u(r, \phi) |_{\phi = \pm \phi_0}, \tag{B5}$$

for any $r > 0$ and $h'(x) = \alpha = \tan \phi_0$.

This task is related to the calculation of the 2D stationary density of particles dragged out of the cone by a constant force along the $x$ axis. If we rotate our channel in Fig. 3 by $\pi/2$, we get the relevant picture, Fig. 6. In comparison to the previous problem, the particles diffuse in a different sector; instead of the angle $\psi = \phi + \pi/2 \in (0, \pi/2 - \phi_0)$, they are confined in $\psi \in (\pi/2 - \phi_0, \pi/2 + \phi_0)$. For certain values of $\phi_0$, we can extend the known solutions in the sector adjacent to the $x$ axis to the sector of our interest.

We recall briefly the stationary solution of the Smoluchowski equation in the sector $\psi \in (0, \phi_0)$. After rotation of the coordinate system, $\phi$ is simply replaced by $\psi$ in Eq. (3.3) and the rotated BC (3.5),

$$\partial_\psi u(r, \psi) = -\frac{gr}{2} \sin(\psi)u(r, \psi) \tag{B6}$$

has to be satisfied at $\psi = \pm \psi_0$. To express the solutions $u(r, \psi)$ here, we are inspired by the integral representation of the Bessel functions $K_\nu$, \[K_\nu(r) = \int_0^\infty e^{-r \cosh t} \cosh \nu t \, dt \tag{B7}\]

One can check by direct calculation, that the integral

$$u(r, \psi) = \int_0^\infty e^{-(gr/2) \cosh t} \left[f(t + i\psi) + f(t - i\psi) \right] dt \tag{B8}$$

is a solution of the equation (with $\phi$ replaced by $\psi$) for any even analytic function $f(z) = f(-z)$ of the complex variable $z$ having no pole along the integration path. Notice also that the function (B8) has expected symmetry $u(r, \psi) = u(r, -\psi)$, given by the direction of the force along the $x$ axis.

The function $f(z)$ is fixed from the BC at $\psi = \pm \psi_0$. Applying the formula (B8) in Eq. (B6) and integrating by parts, we obtain the condition

$$[f(t + i\psi_0) - f(t - i\psi_0)] \sinh t =$$

$$= i[f(t + i\psi_0) + f(t - i\psi_0)] \sin \psi \tag{B9}$$

valid for any $t \geq 0$. If we write $f(z) = g(z) \tanh(z/2)$, $g(z)$ has to satisfy $g(t + i\psi_0) = g(t - i\psi_0)$. Then the "ground state" solution $u_0(r, \psi)$ is generated by $g_0(z) = \coth(\pi z/2\psi_0)$ and the other particular solutions $u_n(r, \psi)$ come from $g_n(z) = \sinh(n\pi z/\psi_0)$. Again, only $u_0(r, \psi)$ is connected with the 1D stationary flux flowing along the $x$ axis, and $u_{2n+1}$ are modes projected out by the mapping procedure (17), which are not necessary for calculation of $D(x)$.

To get the solution $u_0$ for the cone with the transverse field, i.e. for the sector $\psi \in (\pi/2 - \phi_0, \pi/2 + \phi_0)$, we have to find the function $f(z)$ such that the BC (16) are satisfied at $\psi = \pi/2 \pm \phi_0$. The same treatment leads to a condition similar to Eq. (B9): if we write $f(z) = g(z) \tanh(z/2)$, then $g(t + i\psi) = g(t - i\psi)$ is required at both boundaries, $\psi = \pi/2 \pm \phi_0$, and any $t \geq 0$.

For specific angles $\phi_0$, we can adopt the function

$$g_0(z) = \coth(mz/2) = \frac{e^{\text{mz}} + 1}{e^{\text{mz}} - 1}. \tag{B10}$$

It satisfies the required condition not only at $\psi_0 = \pi/m$, used in the sector adjacent to the $x$ axis, but also at any its integer multiple. To get the "ground state", we need to adjust $\pi/2 \pm \phi_0$ to be succeeding integer multiples of $\pi/m$; the imaginary part of $m(t + i\psi)$ has to change by $i\pi$ if $\psi$ increases from $\pi/2 - \phi_0$ up to $\pi/2 + \phi_0$. These requirements are met for odd numbers $m \geq 3$. For the corresponding angles $\phi_0 = \pi/m = \pi/6, \pi/10, \ldots$, the formula (B10) becomes the function $g_0(z)$ generating the "ground state" $u_0(r, \psi)$ also in the sector of our interest.

Still, there is a problem at the boundary whose angle $\psi$ is an even multipule of $\psi_0$; the function $g_0(z)$ and also the corresponding $f(z)$ have a pole at $t = 0$. We solve it by changing the integration path in the complex plane.

First we return back to the unrotated coordinate system and the angle $\phi$. The variable $t$ in the integral (B8),

$$u(r, \phi) = \int_0^\infty e^{-(gr/2) \cosh t} \left[ f(t + i\phi + i\pi/2) + f(t - i\phi - i\pi/2) \right] dt \tag{B11}$$

can be substituted by $t = z \pm i\pi/2$ and the path is then shifted in the complex plane by $\mp i\pi/2$ correspondingly. In the final formula, rewritten in a symmetric way,

$$2u(r, \phi) = \int_0^{i\pi/2 + \infty} e^{-(gr/2) \cosh(z - i\pi/2)} \left[ f(z + i\phi)$$

the term proportional to $C$ integrates solves the equation (B3) for any $f$ function (B10) satisfies these conditions for $\phi$ correction of the force (Fig. 3). Direct calculation shows $\rho$ density results in the conditions ing Eq. (B12) in the BC (B5) and integrating by parts which has no pole along the integration path. Substitution path in both integrals avoids the poles at $z$ in influences the calculation of specific slopes $\alpha_{\pm}$ we change the lower limits in Eq. (B12), we obtain the "ground state" solution $u_{0}(r, \phi)$ in the linear cone with a transverse force for these $\pm \phi = \pm \phi_{0}$ and any $z$ on the integration path; Substituting Eq. (B12) in the BC (B5) and integrating by parts results in the conditions $g(z \pm i\phi) = g(z \mp i\phi \mp i\pi)$ at $\phi = \pm \phi_{0}$ and any $z$ on the integration path; we rewrote again $f(z) = g(z) \tanh(z/2)$. It is easy to verify that the function (B11) satisfies these conditions for $\phi_{0} = \pi/2m$, $m = 3, 5, ...$, so taking

$$f(z) = \coth(mz/2) \tanh(z/2)$$  \hfill (B13)

in Eq. (B12), we obtain the "ground state" solution $u_{0}(r, \phi)$ in the linear cone with a transverse force for these specific slopes $\alpha = \tan \phi_{0}$.

In the resultant stationary density, two integration constants can be added,

$$\rho(x, y) = C_{1} e^{-gy/2} u_{0}(x, y) + C_{0} e^{-gy}.$$  \hfill (B14)

$C_{1}$ controls the stationary net flux connected with the density $\rho(x, y)$ and $C_{0}$ sets the BC $\rho(x, y) = 0$ at a distant boundary absorbing the particles. None of them influences the calculation of $D(x)$. The contribution of the term proportional to $C_{0}$ to $p(x)/A(x)$ is constant and so it gives zero in the formula (3.5). The net flux $J$, as well as $\partial_{x}[p(x)/A(x)]$, are proportional to $C_{1}$ and so it is canceled in the resultant $D(x)$.