Phase space reduction of the one-dimensional Fokker-Planck (Kramers) equation

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I. INTRODUCTION

The Brownian motion of a particle in a confined system represents an essential model used in description of stochastic transport through quasi one-dimensional (1D) systems, e.g. channels in nanomaterials, pores or fibers in biological structures. In a 1D system, the trajectory $x(t)$ of a Brownian particle is described by the Langevin equation

$$m\ddot{x} + \gamma \dot{x} + \partial_x U(x) = f(t).$$

Here, $m$ denotes mass of the particle, $U(x)$ represents the driving potential, $\gamma$ is an effective friction coefficient and $f(t)$ is the stochastic force, satisfying the usual conditions on average values, $\langle f(t) \rangle = 0$ and $\langle f(t)f(t') \rangle = 2\gamma k_B T \delta(t-t')$. $T$ is the temperature and $k_B$ the Boltzmann constant. The corresponding phase space density $\rho(x,v,t)$ of the particle satisfies the Fokker-Planck (FP), or Kramers (kinetic) equation,

$$\left(\partial_t + v \partial_x - \frac{U'(x)}{m} \partial_v\right) \rho(x,v,t) = \frac{\gamma}{\beta m^2} \partial_v e^{-\beta mv^2/2} \partial_v e^{\beta mv^2/2} \rho(x,v,t),$$

where $x$ is the spatial coordinate, $v$ denotes its velocity and $\beta = 1/k_B T$ is the inverse temperature.

Solutions of the Langevin equation, as well as the corresponding kinetic equation, are studied over almost a century \cite{1,2}. Still, motion of a particle in confined geometries represents usually a complicated problem, requiring next reductions of the used description. Due to simplicity, and often for relevance, mainly the overdamped limit is studied. The mass dependent term in Eq. (1.1), $m\ddot{x}$, is then considered negligible and the particle’s spatial density $\rho(x,t)$ is governed by the Smoluchowski equation,

$$\partial_t \rho(x,t) = D_0 \partial_x e^{-\beta U(x)} \partial_x e^{\beta U(x)} \rho(x,t),$$

containing no information about the mass of the particle; $D_0$ denotes the diffusion constant. Instead of the full phase space, one works with only the spatial coordinate $x$. Of course, the question is the price for this simplification, as well as possibility of also including properly inertia of the massive particles in the reduced (real space only) description of the Brownian dynamics. Recent studies showed its importance in understanding rectification of the transport in ratchets \cite{4}, or its influence on the effective diffusion coefficient \cite{5-7} in a narrow channel. For our purpose to demonstrate the phase space reduction, we will deal here with only the 1D FP (Kramers) equation (1.2).

The eq. (1.2) is reducible to the Smoluchowski eq. (1.3) in the limit $m \to 0$. The reduction procedure \cite{5-7} is based on an instant thermalization of the particle’s velocity after any move in the $x$ direction in the case of an infinitely small mass. The situation resembles derivation of the Fick-Jacobs (FJ) equation \cite{11,12},

$$\partial_t \rho(x,t) = \partial_x A(x) \partial_x \frac{\rho(x,t)}{A(x)},$$

appearing as the result of the dimensional reduction of the diffusion equation in a 2D channel with varying cross section $A(x)$, onto the longitudinal coordinate $x$, if equilibration in the transverse ($y$) direction is instant. The function $\rho(x,t)$ denotes the linear (1D) density of the particle. Of course, as in reduction of diffusion to the FJ equation, that of (1.2) to (1.3) as $m \to 0$ is a singular limit, and must be handled with care, but from the viewpoint of the reduction of (1.1), no such caveat is needed.

Recently, an exact mapping procedure was proposed \cite{13,14}, enabling us to also derive the corrections to the FJ equation (1.3), which are necessary, if the transverse equilibration is not instant. The key was to introduce anisotropy of the diffusion constant in the diffusion equation,

$$\partial_t \rho(x,y,t) = \left(\partial_x^2 + \frac{1}{\epsilon} \partial_y^2\right) \rho(x,y,t),$$

where $\epsilon$ is the epsilon function which should vanish in the $y \to 0$ limit.
governing the 2D (spatial) density $\rho(x, y, t)$. For $\epsilon \to 0$, the infinitely fast transverse diffusion immediately flattens the $y$ profile of $\rho(x, y, t) \to \rho(x, t) = \rho(x, t)/A(x)$. Then integration of Eq. (1.5) over the cross section, together with the reflecting boundary conditions satisfied at the hard walls, results in the FJ eq. (1.4). In the case of a slower transverse diffusion, the mapping procedure generates a series of corrections to the FJ equation controlled by $\epsilon > 0$, developing the $y$ profile of $\rho(x, y, t)$, which is already curved depending on the flux and geometry of the channel.

The procedure was extended to mapping of diffusion in an external field $U(x, y)$, e.g. for diffusion in a channel with soft walls [13], where the particle is kept near the $x$ axis by the parabolic potential, $\beta U(x, y) = \alpha(x)y^2$; $\alpha(x)$ represents the varying stiffness of the walls. The equation to be mapped onto the $x$ coordinate is the 2D Smoluchowski equation,

$$\left(\partial_t - \partial_x e^{-\alpha(x)y^2} \partial_x e^{\alpha(x)y^2}\right) \rho(x, y, t) = \frac{1}{\gamma} \partial_y e^{-\alpha(x)y^2} \partial_y e^{\alpha(x)y^2} \rho(x, y, t). \quad (1.6)$$

Integrating over $y$ and applying the mapping scheme gives the mapped 1D equation in an extended Smoluchowski form,

$$\partial_t p(x, t) = \partial_x e^{-V(x)} \left[1 + \epsilon \hat{Z}(x, \partial_x)\right] \partial_x e^{V(x)} p(x, t), \quad (1.7)$$

governing the 1D density $p(x, t)$, where $V(x)$ stands for an effective potential and $\hat{Z}$ is the correction operator sought as an expansion in the small parameter $\epsilon$. The potential $V(x)$ and the coefficients of $\hat{Z}$ depend on $\alpha(x)$ and both are fixed unambiguously within the recurrence mapping procedure.

The central idea of this paper is a conjecture that the FP eq. (1.2) can be reduced to an extended Smoluchowski-like 1D form, governing the spatial density $p(x, t)$, after integration over $v$ and applying a similar mapping scheme. The velocity $v$ thus represents a “transverse” coordinate instead of $y$, with the mass $m$ playing the role of the small parameter $\epsilon$. Then the Smoluchowski equation (1.3) should be obtained in the limit $m \to 0$ [13]. Performing the recurrence procedure, a series of corrections to this equation in powers of $m$ would be derived. Then the final mapped equation would also respect inertia of the Brownian particles, although working only in real space.

Use of the mapping procedure developed for diffusion [13, 16] is not straightforward; the left-hand side operator of the FP equation (1.2) has a different structure than that of the diffusion (1.5) or Smoluchowski equation (1.3). Still, there is a way to apply the general scheme of the mapping in this case and to perform reduction of the phase space onto the real space in the way described above. Presentation of this algorithm is the primary aim of this study.

The result of the mapping of the FP equation (1.2) is again an equation of the form (1.7) with $V(x) = \beta U(x)$ and $\epsilon$ replaced by $m$. In the limit of stationary flow, this equation can be simplified by subsequent reduction of the operator $1 - m\hat{Z}$ to a function $D(x)$, a spatially dependent effective diffusion coefficient [12, 17],

$$\partial_t p(x, t) = \partial_x e^{-\beta U(x)} D(x) \partial_x e^{\beta U(x)} p(x, t). \quad (1.8)$$

The leading term of $D(x)$ is proportional to $mU''(x)$ and the whole series of corrections to the Smoluchowski equation can be summed up, giving

$$D(x) = D_0 \frac{1 - \sqrt{1 - 4mU''(x)/\gamma^2}}{2mU''(x)/\gamma^2}, \quad (1.9)$$

with $D_0 = 1/\gamma \beta$, if the higher derivatives of $U(x)$ are neglected.

In the following section, we analyze how to apply the mapping scheme for reduction of the phase space in the FP equation (1.2). In Sect. III, our considerations are verified on an exactly solvable model, the FP equation with no field, $U(x) = 0$. Analysis of this example helps us to construct the recurrence scheme for calculation of the series of corrections to the zeroth order approximation, the Smoluchowski eq. (1.3), in the small parameter $m$. Finally, the complete mapping procedure for an arbitrary potential $U(x)$ is presented in Sect. IV. The mapped equation of type (1.7), as well as the formula (1.9) is derived, and checked on the damped linear harmonic oscillator.

II. PRELIMINARY CONSIDERATIONS

The key points of the mapping procedure, as formulated for diffusion [13, 14], are recalled in this Section. Based on physical considerations, we adjust the general scheme of the mapping for dimensional reduction of the FP equation (1.2) to this situation.

The mapping procedure represents a consistent transition from a fine grain to a coarse grain description of some evolution process. The process is described in details by some partial differential equation (PDE), governing the density of particles $\rho(r, t)$ in the full space, defined by the coordinates $r$. The dimensional reduction projects this equation onto another PDE, which governs the density $p(x, t)$ in the reduced space of the coordinate $x$. The coordinate $x$ is one of the coordinates of the full space, $r = (x, y)$, and the mapping accomplishes integration over the transverse coordinates $y$. In the case of the FP equation (1.2), phase space $(x, v)$ represents the full space and the dimensional reduction integrates over the “transverse” coordinate, the velocity $v$. Hence we have the defining relation between the densities $\rho$ and $p$:

$$p(x, t) = \int_{-\infty}^{\infty} \rho(x, v, t) dv. \quad (2.1)$$
The phase-space density \( \rho(x,v,t) \) is expected to be near the thermodynamic equilibrium and so approximately proportional to \( \exp(-\beta mv^2/2) \), which provides convergence of the integral in Eq. (2.4).

Then the first step of the mapping is also integration of Eq. (1.2) over \( v \). If completed, we get

\[
\int_{-\infty}^{\infty} (\partial_t + v \partial_x) \rho(x,v,t) dv = 0; \quad (2.2)
\]

the other terms are zero due to \( \rho(x,v,t) \to 0 \) in the limit \( v \to \pm \infty \). This equation represents nothing but mass conservation in the reduced space,

\[
\partial_t p(x,t) + \partial_x j(x,t) = 0, \quad (2.3)
\]

where the 1D flux \( j \) is defined by the relation

\[
\int_{-\infty}^{\infty} v p(x,v,t) dv = j(x,t). \quad (2.4)
\]

In contrast to diffusion, where \( j = -D_0 \partial_x p \) is fixed, here the flux \( j \) is a function formally independent of the density \( p \), so we also need the evolution equation for this quantity. After integration of Eq. (1.2) multiplied by \( v \), we obtain

\[
\partial_t j(x,t) + \partial_x \int_{-\infty}^{\infty} v^2 \rho(x,v,t) dv + \frac{U'(x)}{m} p(x,t) = -\frac{\gamma}{\beta m} \int_{-\infty}^{\infty} e^{-\beta mv^2/2} \rho(x,v,t) dv \quad (2.5)
\]

[after some algebra and applying the definitions (2.1) and (2.4)]. This step recalls the Grad’s method of moments [18, 19]. For the 1D Kramers equation (1.2), taking only a couple of the zeroth (\( p \)) and the first (\( j \)) order moment of the phase space density \( \rho \) is satisfactory for generating the selfconsistent system of the mapped (real space) equations (2.3) and (2.5).

The next key point of the mapping algorithm is that of expressing the full-space density \( \rho(x,v,t) \) using the 1D density \( p(x,t) \) and also the flux \( j(x,t) \) in this case. This relation enables us to complete integrations in Eq. (2.5) and get the evolution equation for \( j(x,t) \), together with the 1D mass conservation, in closed form. The initial task is to find the zeroth order approximation, valid in the limit \( m \to 0 \). Our first proposal for such a relation between \( \rho(x,v,t) \) and the reduced space quantities \( p \) and \( j \) is based on the following physical construction:

For an infinitely small mass of the particle, the stochastic force thermalizes its velocity \( v \) almost immediately after any move along the spatial coordinate \( x \). Similar to the transverse equilibration of the 2D density of a particle diffusing in a narrow channel with biasing transverse force [13, 20, 22], one could try the formula with separated Boltzmann factor in the fast relaxing "direction" \( v \), \( \rho(x,v,t) \approx \sqrt{3m/2\pi p(x,t)} \exp(-\beta mv^2/2) \). It is easy to check that it does not work here; the flux \( j \) becomes zero according to Eq. (2.4). To prevent this failure, let us suppose that the distribution in \( v \) is shifted by the local mean (macroscopic) velocity \( v_0 \), depending on the local flux, \( j(x,t) = v_0(x,t)p(x,t) \). Then we have

\[
\rho(x,v,t) \approx \sqrt{\frac{3m}{2\pi}} e^{-\beta(mv-v_0)^2/2} p(x,t) \approx \sqrt{\frac{3m}{2\pi}} [1 + \beta mv_0 + ...] e^{-\beta mv^2/2} p(x,t).
\]

Retaining only these two terms in the square brackets and replacing \( \rho_0 p \) by the flux \( j \), one gets

\[
\rho_0(x,v,t) = \sqrt{\frac{3m}{2\pi}} e^{-\beta mv^2/2} [p(x,t) + \beta m v j(x,t)], \quad (2.6)
\]

which will be taken as the sought zeroth order relation between \( \rho \) and the reduced space quantities, \( p \) and \( j \).

This heuristic formula will be verified later by the exact mapping algorithm. Still, one can check immediately that the relation (2.6) represents correctly a kind of backward mapping of the 1D (spatial) functions \( p \) and \( j \) onto the phase space densities \( \rho \); if substituted for \( \rho(x,v,t) \) in the defining relations (2.1) and (2.4), we obtain identities. Applying Eq. (2.6) to Eq. (2.5), the integrals over \( v \) can be completed and the result,

\[
\partial_t j(x,t) + \partial_x \left( \frac{p(x,t)}{\beta m} + \frac{U'(x)}{m} p(x,t) \right) = -\frac{\gamma}{\beta m} j(x,t), \quad (2.7)
\]

together with the mass conservation, Eq. (2.3), forms a closed couple of PDE, governing the mapped quantities \( p \) and \( j \).

In the limit \( m \to 0 \), the first term in Eq. (2.7), \( \partial_t j \), becomes negligible and the equation expresses the zeroth order relation between the flux \( j \) and the density \( p \),

\[
j(x,t) = -\frac{1}{\beta \gamma} e^{-\beta U(x)} \partial_x e^{\beta U(x)} p(x,t). \quad (2.8)
\]

If combined with the mass conservation, Eq. (2.3), we get the Smoluchowski equation (1.3); \( 1/\beta \gamma = D_0 \) represents the diffusion constant.

The calculation presented shows that the Smoluchowski equation (1.3) is related to the FP equation (1.2) in the same way as the Fick-Jacobs equation (11) to the diffusion equation valid in a narrow 2D channel. Both mapped equations describe an asymptotic behavior of the full-space density infinitely rapidly equilibrating in the transverse direction; the velocity \( v \) plays the role of the transverse coordinate for the FP equation. Our considerations indicate that the mass of the particle, \( m \), becomes the small parameter, controlling the series of corrections to the Smoluchowski equation in the case when the transverse equilibration is not infinitely fast.

Following the scheme of the mapping procedure [1, 14], the next point is that of searching for the true relation between the phase space density \( \rho(x,v,t) \) and the
1D quantities $p(x, t)$ and $j(x, t)$, replacing the heuristic formula (2.6), valid for nonzero $m$. Without losing generality, it can be written in the form

$$
\rho(x, v, t) = \frac{\sqrt{3m}}{2\pi} e^{-\beta mv^2/2} \left[ \hat{\omega}(x, v)p(x, t) + \beta mv \hat{\eta}(x, v)j(x, t) \right]. \quad (2.9)
$$

If the operators $\hat{\omega}$ and $\hat{\eta}$ (with $\partial_x$ implicit) are expandable in $m$, one can substitute for $\rho(x, v, t)$ in the FP equation (1.2) and fix the coefficients of these operators to satisfy this equation in each order of $m$, similar to the mapping of diffusion. Then, using the relation of backward mapping (2.9) in Eq. (2.5) gives the expansion of the diffusion equation for $\hat{\omega}$ and finally, in combination with mass conservation (2.3), the sought series of corrections to the Smoluchowski equation (1.3) in terms of the finite mass $m$.

To verify whether this scheme is viable, we analyze the exactly solvable case with $U(x) = 0$ in the next Section.

### III. EXACTLY SOLVABLE MODEL

The exact solution of the FP equation (1.2) with no potential, $U(x) = 0$, is presented in this Section. We demonstrate the mapping on the example of the phase space density $\rho(x, v, t)$ evolving from the initial density $\rho(x, v, 0)$ with thermalized velocity $v$. The mapped equation, as well as the form of the operators $\hat{\omega}$ and $\hat{\eta}$ in Eq. (2.9), can be found explicitly in this case. This analysis will direct us in construction of the recurrence mapping scheme in Sect. IV.

The case $U(x) = 0$ is exactly solvable [23], the Green’s function $G(x, v, t; x', v', t')$ of the FP equation (1.2),

$$
\left[ \partial_t + v \partial_x - \frac{\gamma}{\beta m^2} \partial_x e^{-\beta mv^2/2} \partial_v e^{\beta mv^2/2} \right] G(x, v, t; x', v', t') = \delta(x - x') \delta(v - v') \delta(t - t'),
$$

(3.1)
can be derived explicitly (see Appendix A),

$$
G = \frac{\gamma}{4\pi} \frac{\Theta(\tau - \tau')}{\sqrt{\tau - \tau' - \tanh(\tau - \tau')} \sqrt{1 - q^2}} \times \exp \left( -\frac{q}{4} \frac{[2(\xi - \xi') - (u + u') \tanh(\tau - \tau')]^2}{\tau - \tau' - \tanh(\tau - \tau')} \right),
$$

(3.2)

if expressed in the scaled coordinates,

$$
\begin{align*}
\tau &= \gamma t / 2m, \\
\xi &= (\beta m/2)^{3/2} \frac{\gamma x}{\beta m^2}, \\
u &= \sqrt{\beta m / 2} v,
\end{align*}
$$

(3.3)

and $q = \exp[-2(\tau - \tau')]$. If the thermalized particle is inserted at time $t = 0$ with a spatial distribution $p_0(x)$,

$$
\rho(x, v, 0) = \sqrt{\frac{3m}{2\pi}} p_0(x) e^{-\beta mv^2/2}, \quad (3.4)
$$
evolution of the density $\rho$ is given by the formula

$$
\begin{align*}
\rho(x, v, t) &= \sqrt{\frac{3m}{2\pi}} \int_{-\infty}^{\infty} dv' \int dx' G(x, v, t; x', v', 0) \\
&= \int \frac{p_0(x') dx'}{4\pi D_0 \sqrt{Z}} \exp \left( -\frac{[\xi - \xi']^2}{Q}\right)
\end{align*}
$$

(3.5)

$$
D_0 = 1/\gamma \beta, \quad \text{the abbreviations}
$$

$$
\begin{align*}
Q &= \tau - \frac{1}{2} (1 - e^{-2\tau}), \\
Z &= Q - \frac{1}{4} (1 - e^{-2\tau})^2
\end{align*}
$$

(3.6)

are used and the integration over $x'$ runs over the whole (unspecified) 1D spatial domain.

Then the spatial (1D) density $p$ and the flux $j$ are integrated directly according to Eqs. (2.1) and (2.2),

$$
\begin{align*}
p(x, t) &= \sqrt{\frac{2}{3m}} \int \frac{p_0(x') dx'}{4D_0 \sqrt{Q}} e^{-(\xi - \xi')^2/Q}, \\
\frac{1}{2} j(x, t) &= \sqrt{\frac{2}{3m}} \int \frac{p_0(x') dx'}{8D_0 \sqrt{Q} 4Q} (1 - e^{-2\tau}) \times (\xi - \xi') e^{-(\xi - \xi')^2/Q}.
\end{align*}
$$

(3.7)

It is easy to check that the mass conservation (2.3), $\partial_x p + \sqrt{3m/2} \partial_x j = 0$ in the scaled coordinates, is satisfied. The quantity $Q$ plays the role of a “stretched” time [24]. For short times, $t \ll 2m/\gamma$, $Q \approx \tau^2$ and $Z \approx 4\tau^2/3$. The formulas (3.5) and (3.7) describe correctly behavior of the Newtonian particles in this limit. The mapping procedure, as outlined in the previous Section, requires us to study asymptotic behavior in the opposite limit, $t \gg 2m/\gamma$.

For large times, $\tau \to \infty$, the stretched time $Q$ becomes $\tau$ and the formulas (3.7) represent the general solution of the diffusion equation, as expected according to the previous Section. Now it is necessary to verify that the mass $m$ can serve as a small parameter controlling the series of corrections to the diffusion equation and its solution. It may look problematic at first glance, because $Q$ contains $\exp(-2\tau) = \exp(-\gamma t/m)$, representing essential singularity of the variable $m \to 0$. Then the formulas (3.7) [and similarly Eq. (3.5)] are not expandable in $m$. Nevertheless, this property is still consistent with the general scheme of the mapping, as analyzed in Ref. [14].

The dimensional reduction, as demonstrated on anisotropic diffusion in a narrow channel [13], also reduces the Hilbert space of the full-space problem. Let us
denote $\tilde{M}(\epsilon)$ the spatial operator of the evolution equation, i.e. $M(\epsilon) = \partial^2_x + (1/\epsilon)\partial^2_t$ for anisotropic 2D diffusion; the eigenvalues $\lambda_i$ and the eigenfunctions $\psi_i(x,y)$ are given by the equation

$$-\tilde{M}(\epsilon)\psi_i(x,y) = \lambda_i(\epsilon)\psi_i(x,y), \quad (3.8)$$

supplemented by proper boundary conditions at the walls of the channel. The parameter of anisotropy $\epsilon < 1$ splits the spectrum into two parts, the low-lying states, whose eigenvalues $\lambda_i(\epsilon)$ remain finite for $\epsilon \to 0$ and the transients with $\lambda_i(\epsilon)$ diverging $\sim 1/\epsilon$. Then the exact 2D density $\rho$ evolves as

$$\rho(\epsilon; x, y, t) = \sum_i c_i\psi_i(\epsilon; x, y)e^{-\lambda_i(\epsilon)t}, \quad (3.9)$$

the constants $c_i$ are given by the initial condition and the summation runs over the whole spectrum. The transients contribute to the sum by the terms proportional to $\exp(-\lambda_i t/\epsilon)$, where $\lambda_i = \epsilon\lambda_i(\epsilon)$ are finite in the limit $\epsilon \to 0$. The result is a formula containing the essential singularity in the parameter $\epsilon$ near zero, similar to Eq. (3.9) with singular exp($-\gamma t/m$) for $m \to 0$.

The mapping procedure reduces the full Hilbert space of all $\psi_i$ onto the space defined only by the low-lying states $\psi_i$. If the 1D density $p(x,t)$ is integrated from Eq. (3.9) and mapped backward onto the full Hilbert space (by some operator $\hat{\omega}$), the transients will be canceled; the sum runs only over the low-lying states $\psi_i$. The terms retained involve no essential singularity in $\epsilon$; the formula for $\rho$ considered in the mapping procedure represents the regular part of the exact 2D density $\rho$ with respect to the parameter $\epsilon$ near zero. This reduction is natural for the zero-th order (Fick-Jacobs) approximation, as the transients decay infinitely fast due to their infinite eigenvalues $\lambda_i(\epsilon \to 0)$. Nevertheless, the mapping based on fixing the series of corrections expanded in $\epsilon$ can work only with the regular part of the 2D density.

Correspondingly, the formulas (3.10) and (3.11) are exact, including the contributions of the transients, which are represented by the singular terms $\sim \exp(-\gamma t/m)$. The mapping requires us to analyze only the regular parts,

$$p_{reg}(x,t) = \int \frac{p(x')dx'}{2\sqrt{\pi D_0(t-D_0\beta m)}} \times \exp \left[-\frac{(x-x')^2}{4D_0(t-D_0\beta m)}\right],$$

$$j_{reg}(x,t) = \int \frac{\partial_x p(x')dx'}{4\sqrt{\pi D_0(t-D_0\beta m)^2}} \times \exp \left[-\frac{(x-x')^2}{4D_0(t-D_0\beta m)}\right], \quad (3.10)$$

and

$$\rho_{reg}(x, v, t) = \sqrt{\frac{2m}{2\pi}} \int \frac{p(x')dx'}{2\sqrt{\pi D_0(t-3D_0\beta m/2)}} \times \exp \left[-\frac{(x-x')^2}{4D_0(t-3D_0\beta m/2)} - \frac{1}{2}\beta mv^2\right], \quad (3.11)$$

written in the unscaled coordinates, obtained after taking only the regular parts of $Q$ and $Z$ (3.0). $Q_{reg} = \tau - 1/2$ and $Z_{reg} = \tau - 3/4$, in Eqs. (3.7) and (3.5). Of course, the formulas are applied for $t \gg D_0\beta m$, when the transients vanish. We omit writing the subscript ”reg” in the following text.

In comparison with the overdamped limit $m \to 0$, evolution of the spatial (1D) density $p$ and the flux $j$ is only corrected by a time shift, $t \to t - D_0\beta m$ in the formulas (3.10). The Gaussian distribution is retarded by the time $t_0 = D_0\beta m = m/\gamma$, corresponding to the mean time necessary for losing information about the original velocity. The value of the shift $t_0$ is constant in $x$ and $t$, so the density $p$ (3.10) still obeys the diffusion equation,

$$\partial_t p(x,t) = D_0\partial_x^2 p(x,t), \quad (3.12)$$

and $j(x,t) = -D_0\partial_x p(x,t)$. There is no correction of the zero-th order mapped equation due to the finite mass of the particle. Let us stress that the case of $U(x) = 0$ is extremely simple, similar to the mapping of the 2D diffusion in a flat narrow channel, also giving no corrections to the Fick-Jacobs approximation.

Nevertheless, the relation of the backward mapping, generating the phase-space density $\rho$ from the mapped quantities $\hat{p}$ and $\hat{j}$, is not quite trivial. In the formula for $\rho$, Eq. (3.11), the time is shifted by $3t_0/2$ and the displacement $x-x'$ by $vt_0$ with respect to the distribution of a massless particle. The shortest way to construct the relation of backward mapping is by applying the shift operators in $t$ and $x$ on $p(x,t)$, compensating the different shifts of time and displacement in Eqs. (3.10) and (3.11),

$$\rho(x, v, t) = \sqrt{\frac{2m}{2\pi}} e^{-\beta mv^2/2} e^{-(t_0/2)\partial_t - vt_0\partial_x} p(x,t). \quad (3.13)$$

Due to Eq. (3.12), the operator $\partial_t$ in the exponent can be replaced by $D_0\partial_x^2$. After expanding the shift operator $e^{-vt_0\partial_x}$ and using $j = -D_0\partial_x p$, we arrive at the relation of the form (2.9),

$$\rho(x, v, t) = \sqrt{\frac{2m}{2\pi}} e^{-\beta mv^2/2 - (D_0t_0/2)\partial_x^2} \sum_{k=0}^{\infty} (\beta mv^2)^k \times (D_0t_0)^k \partial_x^k \left\{ \frac{1}{(2k)!} p(x,t) + \frac{\beta mv^2}{(2k + 1)!} j(x,t) \right\}. \quad (3.14)$$

the explicit formulas for $\hat{\omega}$ and $\hat{n}$ to be substituted in Eq. (2.9) in the case $U(x) = 0$ are

$$\hat{\omega}(x,v) = e^{-D_0t_0/2} \sum_{k=0}^{\infty} (\beta mv^2)^k (D_0t_0)^k \partial_x^k,$$

$$\hat{n}(x,v) = e^{-D_0t_0/2} \sum_{k=0}^{\infty} (\beta mv^2)^k (D_0t_0)^k \partial_x^k. \quad (3.15)$$
Both operators are expandable in $m$, $(t_0 = m/\gamma)$; their zero-th order coefficients equal unity, consistent with the heuristic formula (2.3). Also applying the relation (3.18) in the definitions (2.11) and (2.4) gives identity.

The final step is that of verifying the evolution equation for $j$, Eq. (2.5). Two integrals are to be completed with $\rho$ expressed by the backward mapping, Eq. (3.14).

\[
\int_{-\infty}^{\infty} v^2 \rho(x, y, t) dv = (1 + D_0 t_0 \partial_x^2) p(x, t)/\beta m, \\
\int_{-\infty}^{\infty} e^{-\beta m v^2/2} \rho(x, v, t) dv = \beta m j(x, t),
\]

which are now valid exactly. If substituted in Eq. (2.5), and the equation (3.12) is applied, we get

\[(1 + t_0 \partial_t) [j(x, t) + D_0 \partial_x p(x, t)] = 0 \quad (3.17)
\]

after simple algebra. This equation validates the relation $j = -D_0 \partial_x p$ for nonzero $m$ as well and thus, if combined with the mass conservation (2.2), also the diffusion equation (3.12) without any corrections. If compared with the calculation of Eq. (2.8), the 1-st order term $\sim \partial_x j$, neglected in the previous Section, is compensated here by other 1-st order term coming from the exact relation (3.18), appearing in the integrals (3.16).

The FP equation (1.2) with zero potential is too simple to give nonzero corrections to the diffusion equation (3.12). Nevertheless, it helped us to understand the structure of the mapping. It shows that the scheme suggested in the previous section is viable. The relation of the backward mapping has the form of Eq. (2.9), at least for $U(x) = 0$, and the operators $\hat{\omega}$ and $\hat{\eta}$ can be expanded in $m$, or $t_0 = m/\gamma$,

\[
\hat{\omega} = \sum_{k=0}^{\infty} t_0^k \hat{\omega}_k(x, u), \quad \hat{\eta} = \sum_{k=0}^{\infty} t_0^k \hat{\eta}_k(x, u). \tag{3.18}
\]

Integration in Eqs. (3.16) indicates that the coefficients $\hat{\omega}_k$ and $\hat{\eta}_k$ should be sought dependent up on the scaled velocity $u$ rather than $v$ (compare to Ref. [24]); otherwise each term in Eq. (3.18) would contribute in several succeeding orders in the integrals (3.16). The mixing of orders would hinder us in constructing the recurrence scheme generating corrections to Eq. (2.5). In the notation of Eq. (3.18), $\hat{\omega}_0 = \hat{\eta}_0 = 1$ and

\[
\hat{\omega}_1(x, u) = (u^2 - 1/2)D_0 \partial_x^2, \\
\hat{\eta}_1(x, u) = (u^2/3 - 1/2)D_0 \partial_x^2, \\
\hat{\omega}_2(x, u) = (u^4/6 - u^2/2 + 1/8)D_0^2 \partial_x^4, \\
\ldots
\]

valid for $U(x) = 0$ according to Eqs. (3.15), will be used for testing the results of the recurrence procedure in the next Section.

\section{IV. MAPPING PROCEDURE}

We now finish the construction of the mapping procedure, outlined in the Section II, for an arbitrary analytic potential $U(x)$. Supposing the backward mapping of the form (2.9) with the operators $\hat{\omega}$ and $\hat{\eta}$ expanded in $t_0$ ($m$) according to Eqs. (3.18), we find recurrence relations fixing the coefficients $\hat{\omega}_k$ and $\hat{\eta}_k$. Completing the integrals in Eq. (2.5), we obtain a series of corrections to the zero-th order relation $j = -D_0 \partial_x p$. Combined with mass conservation, Eq. (2.3), it gives the Smoluchowski equation corrected due to nonzero mass of the particle.

The essential relation determining the operators $\hat{\omega}$ and $\hat{\eta}$ is the FP equation (1.2), which has to be satisfied for any solution of the reduced problem, the density $p(x,t)$ and the flux $j(x,t)$, after their backward mapping (2.9) onto the full-dimensional Hilbert space. If the expansion in $t_0 = m/\gamma$ of both operators, Eq. (3.18), is supposed, we have

\[
\left[ \partial_t + \sqrt{\frac{2}{\beta m}} u \partial_x - \beta U'(x) \partial_u - \frac{1}{2t_0} e^{-u^2} \partial_u e^{u^2} \right] \sum_{k=0}^{\infty} t_0^k \times e^{-u^2} \left[ \hat{\omega}_k(x, u) p(x, t) + \sqrt{2\beta m u} \hat{\eta}_k(x, u) j(x, t) \right] = 0 \quad (4.1)
\]

after introducing the scaled velocity $u = \sqrt{\beta m/2\nu}$ in Eq. (1.2). The factor $\beta m$ is replaced by $t_0/D_0$ in the following calculations. Thus half-integer powers of $t_0$ appear in Eq. (4.1) [24]. As this equation has to be satisfied for any $t_0$, we can split it for clarity into two relations: the first one, including only the integer powers of $t_0$,

\[
\sum_{k=0}^{\infty} t_0^k \left[ \partial_t \omega_k p + 2u^2 \partial_u \eta_k j - \beta U'(x) e^{u^2} \partial_u e^{-u^2} \eta_k j \right.
\]

\[
\left. - \frac{1}{2t_0} e^{u^2} \partial_u e^{-u^2} \partial_u \omega_k p \right] = 0, \tag{4.2}
\]

and the second one, collecting the half-integer powers,

\[
\sum_{k=0}^{\infty} t_0^{k-1/2} \left[ 2t_0 u \partial_t \eta_k j + D_0 \left( 2u \partial_x - \beta U'(x) e^{u^2} \partial_u e^{-u^2} \right) \right.
\]

\[
\left. \times \omega_k p - e^{u^2} \partial_u e^{-u^2} \partial_u \eta_k j \right] = 0. \tag{4.3}
\]

Notice that Eqs. (4.2) and (4.3) do not violate parity of $\hat{\omega}_k$ and $\hat{\eta}_k$ in $u$. If used for construction of the recurrence relations between the coefficients, all they have to have the same parity as $\hat{\omega}_0 = \hat{\eta}_0 = 1$; hence $\hat{\omega}_k(x, u) = \hat{\omega}_k(x, -u)$ and $\hat{\eta}_k(x, u) = \hat{\eta}_k(x, -u)$. This symmetry enables us to find the normalization (or identity) conditions for $\hat{\omega}_k$ and $\hat{\eta}_k$. The backward mapped $\rho$, Eq. (2.9), with the operators $\hat{\omega}$, $\hat{\eta}$ expanded in $t_0$, Eq. (3.18), substituted in the definitions (2.1) and (2.2) has to give identities for any $t_0$, $p(x,t)$ and $j(x,t)$. Thus we obtain

\[
\frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} du e^{-u^2} \hat{\omega}_k(x, u) = \delta_{0,k}, \tag{4.4}
\]
\[ \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} 2u^2 d\omega u^2 \tilde{\eta}_k(x, u) = \delta_{0,k}. \] (4.5)

The operators \( \tilde{\omega}_k \) and \( \tilde{\eta}_k \) are supposed not to depend on time, so the time derivative commutes with them and acts directly on \( p(x, t) \) or \( j(x, t) \) in Eqs. (1.2), (4.3). To derive the operators unambiguously, using only spatial derivatives, we express \( \partial_t p = -\partial_x j \) from the mass conservation, Eq. (2.3). However, the time derivative of \( j \) cannot be expressed in a similar way from Eq. (2.5), because \( \partial_t j \) is not the leading term there. If the backward mapping, Eqs. (2.9) and (3.18), is applied to the integrals of Eq. (2.5), we get

\[ \int_{-\infty}^{\infty} u^2 \rho(x, v, t) dv = \frac{1}{\beta m} \left( 1 + \sum_{k=1}^{\infty} t_k^0 \hat{I}_k(x) \right) p(x, t), \]

where the operators \( \hat{I}_k \) are given by

\[ \hat{I}_k(x) = \frac{2}{\sqrt{\pi}} \int_{-\infty}^{\infty} u^2 d\omega u^2 \tilde{\omega}_k(x, u); \] (4.6)

the right-hand side integral of Eq. (2.3) results in

\[ \frac{\gamma}{\beta m} \int_{-\infty}^{\infty} e^{-\beta m v^2/2} \partial_v e^{\beta m v^2/2} \rho(x, v, t) dv = \frac{\gamma}{\beta m} \sum_{k=0}^{\infty} t_k^0 \int_{-\infty}^{\infty} d\omega \partial_{\omega} u \tilde{\eta}_k(x, u) j(x, t) = \frac{j(x, t)}{t_0} \]

obtained after comparison of Eqs. (4.7) and (4.8). Expanding in \( t_0 \) and comparing the coefficients of the same powers of \( t_0 \), we get a sequence of relations fixing \( \hat{Z}_k \),

\[ e^{-\beta U(x)} \left[ 1 + \sum_{k=1}^{\infty} t_k^0 \hat{Z}_k \right] \partial_x e^{\beta U(x)} = \left[ e^{-\beta U(x)} e^{\beta U(x)} \right] \]

\[ + \partial_x \sum_{k=0}^{\infty} t_k^0 \hat{I}_k \left( 1 + \sum_{k=0}^{\infty} t_k^1 \hat{Q}_k \right)^{-1}, \]

which is to be used in the operator equation,

\[ e^{-\beta U(x)} \left[ \partial_x e^{\beta U(x)} \right] \]

\[ \times \partial_x \sum_{k=0}^{\infty} t_k^0 \hat{Z}_k \partial_x e^{\beta U(x)} = \partial_x \sum_{k=0}^{\infty} t_k^1 \hat{Q}_k \]

\[ + e^{-\beta U(x)} \partial_x e^{\beta U(x)} \left( \hat{Q}_0 - \hat{Q}_1 \right), \]

(4.11)

Finally, we derive the recurrence scheme, generating the operators \( \tilde{\omega}_k \), determining \( \hat{I}_k \), Eq. (4.10), and thus also \( \hat{Z}_k \) or \( \hat{Q}_k \), Eqs. (4.9), (4.11). Notice that the \( \tilde{\eta}_k \) do not directly enter the mapped equation (4.9), but they are necessary in the recurrence formulas for \( \tilde{\omega}_k \).

The recurrence scheme for \( \tilde{\omega}_k \) is defined by Eq. (4.12). This equation has to be satisfied for any \( p \) and \( j \), solving the mapped problem, but these quantities, although considered before as formally independent, are related by Eq. (4.8). To obtain an equation for operators, \( j \) has to be expressed by \( p \). Applying the relation (4.8) and Eq. (4.9) for \( \partial_t p \), we get

\[ \sum_{n=0}^{\infty} t_n^0 \left[ D_0 \left( \tilde{\omega}_n \partial_x - 2u^2 \partial_x \tilde{\eta}_n + \beta U' e^{u^2/2} \partial_x e^{-u^2/2} \tilde{\eta}_n \right) e^{-\beta U(x)} \right] \]

\[ \times \sum_{i=0}^{\infty} t_i^0 \hat{Z}_i \partial_x e^{\beta U(x)} - \frac{1}{2t_0} e^{u^2/2} \partial_x e^{-u^2/2} \partial_x \tilde{\eta}_0 = 0, \] (4.12)

valid for any function \( p(x, t) \); we have \( \hat{Z}_0 = 1 \). To lowest order, \( t_0^{-1} \), only the term \( e^{u^2/2} \partial_x e^{-u^2/2} \partial_x \tilde{\omega}_0 = 0 \). It is satisfied by \( \tilde{\omega}_0 = 1 \), the only solution nondiverging at \( u \to \pm \infty \) and also satisfying the normalization, Eq. (4.3).

In the higher orders, we derive the recurrence relation,

\[ e^{u^2/2} \partial_x e^{-u^2/2} \partial_x \tilde{\omega}_{n+1} = 2D_0 \sum_{k=0}^{n} \left( \tilde{\omega}_k \partial_x - 2u^2 \partial_x \tilde{\eta}_k + \beta U'(x) \right) \]

\[ \times \hat{Z}_n \partial_x e^{\beta U(x)} - \frac{1}{2t_0} e^{u^2/2} \partial_x e^{-u^2/2} \partial_x \tilde{\eta}_0 = 0, \] (4.12)

valid for any function \( p(x, t) \); we have \( \hat{Z}_0 = 1 \). To lowest order, \( t_0^{-1} \), only the term \( e^{u^2/2} \partial_x e^{-u^2/2} \partial_x \tilde{\omega}_0 = 0 \). It is satisfied by \( \tilde{\omega}_0 = 1 \), the only solution nondiverging at \( u \to \pm \infty \) and also satisfying the normalization, Eq. (4.3).

In the higher orders, we derive the recurrence relation,
\[ e^{u^2} \partial_u u e^{-u^2} \hat{\eta}_k \int e^{-\beta U(x)} \hat{Z}_{n-k} \partial_x e^{\beta U(x)} \] (4.13)

Calculation of the \( \hat{\omega}_{n+1} \) requires us to know the \( \hat{\eta}_k \) up to \( k = n \). They are generated from Eq. (4.13). Again, \( j \), as well as \( \partial_j \), have to be expressed by \( y \) using the relations (4.8) and (4.9). Then Eq. (4.13) becomes

\[ \sum_{n=0}^{\infty} t_0^{n-1/2} \left[ e^{u^2} \partial_u e^{-u^2} \partial_u \hat{\eta}_n e^{-\beta U} \sum_{k=0}^{\infty} t_0^k \hat{Z}_k \partial_x e^{\beta U} \right. \\
-2D_0 t_0 u \hat{\eta}_n e^{-\beta U} \sum_{k=0}^{\infty} t_0^k \hat{Z}_k \partial_x e^{\beta U} \\
+ \left. (2u \partial_x - \beta U' e^{u^2} \partial_u e^{-u^2}) \hat{\omega} \right] = 0 \] (4.14)

valid for any function \( p(x, t) \). In lowest order, \( t_0^{-1/2} \),

\[ e^{u^2} \partial_u e^{-u^2} \partial_u \hat{\eta}_0 e^{-\beta U} \partial_x e^{\beta U} = -2u \partial_x + \beta U' e^{u^2} \partial_u e^{-u^2} = -2u (\partial_x + \beta U'') \] (4.15)

where we have used \( \hat{\omega} = 1 \) and \( \hat{Z}_0 = 1 \). After the first integration, we have

\[ \partial_u \hat{\eta}_0 = -e^{u^2} \int 2udue^{-u^2} = 1 + \hat{C}_1 e^{u^2}; \] (4.16)

the integration constant \( \hat{C}_1 = 0 \) provides convergence as \( u \to \pm \infty \). The next integration gives \( \hat{\eta}_0 = 1 + (1/u)\hat{C}_0; \)

\( \hat{C}_0 = 0 \). This calculation validates our heuristic formula (2.6) in the zero-th order approximation.

In the higher orders, Eq. (4.14) generates the relations

\[ e^{u^2} \partial_u e^{-u^2} \partial_u \hat{\eta}_n e^{-\beta U} \partial_x e^{\beta U} = (\beta U' e^{u^2} \partial_u e^{-u^2} - 2u \partial_x) \hat{\omega} + 2D_0 \sum_{k=0}^{n-1} \hat{\eta}_{n-k-1} e^{-\beta U} \hat{Z}_k \partial_x e^{\beta U} \hat{Z}_1 \partial_x e^{\beta U} \\
- \sum_{k=0}^{n-1} e^{u^2} \partial_u e^{-u^2} \partial_u \hat{\eta}_k e^{-\beta U} \hat{Z}_{n-k} \partial_x e^{\beta U}, \] (4.17)

forming the recurrence scheme for \( \hat{\eta}_n \). Completing the operations in Eqs. (4.17) and (4.13) one has to keep in mind that the equation acts on an arbitrary function \( p(x, t) \), not depending on \( u \). On the other hand, the operators \( \hat{\omega}_k \) and \( \hat{\eta}_k \) for \( k > 0 \) depend on \( u \).

The recurrence procedure starts from \( \hat{\omega}_0 = 1 \) and \( \hat{Z}_0 = 1 \). Calculation of the next order correction requires first expressing the \( \hat{\eta}_n \) according to Eq. (4.17), or (4.15) for \( n = 0 \), as shown above. Then \( \hat{\omega}_{n+1} \) is derived from Eq. (4.13), \( \hat{\eta}_{n+1} \) integrated according to Eq. (4.16) and finally \( \hat{Z}_{n+1} \) expressed from Eq. (4.11). To demonstrate the procedure, we derive the first order correction, \( \hat{Z}_1 \).

We use already calculated \( \hat{\eta}_0 = 1 \). For \( n = 0 \), Eq. (4.13) becomes

\[ e^{u^2} \partial_u e^{-u^2} \partial_u \hat{\omega}_1 = 2D_0 (1 - 2u^2) e^{-\beta U(x)} \partial_x^2 e^{\beta U(x)} \] (4.18)

After the first integration,

\[ \partial_u \hat{\omega}_1 = 2D_0 e^{u^2} \left( u e^{-u^2} + C_1 \right) e^{-\beta U(x)} \partial_x^2 e^{\beta U(x)}, \] (4.19)

the integration constant \( C_1 = 0 \), to provide convergence for \( u \to \pm \infty \). The integration constant \( C_0 \) after the next integration is fixed to satisfy the normalization, Eq. (4.14),

\[ \int_{-\infty}^{+\infty} du e^{u^2} D_0 (u^2 + C_0) e^{-\beta U(x)} \partial_x^2 e^{\beta U(x)} = 0, \] (4.20)

hence \( C_0 = -1/2 \) and

\[ \hat{\omega}_1 = D_0 (u^2 - 1/2) e^{-\beta U(x)} \partial_x^2 e^{\beta U(x)}. \] (4.21)

For \( U(x) = 0 \), we recover the corresponding formula in Eq. (3.19). Integration over \( u \) in Eq. (4.10) results in

\[ \hat{Z}_1 = D_0 \left( e^{\beta U} \partial_x e^{-\beta U} \partial_x - \partial_x e^{\beta U} \partial_x e^{-\beta U} \right) = D_0 \beta U''(x) \] (4.22)

from Eq. (4.11).

In the higher orders, \( \hat{\eta}_n, \hat{\omega}_{n+1}, \) and \( \hat{Z}_{n+1} \) are calculated according to Eqs. (4.17) and (4.13). The integration constants after double integration have to provide convergence for \( u \to \pm \infty \), requiring the operators to be even in \( u \), and the normalization, Eq. (4.14). The condition (4.15) for \( \hat{\eta}_n \) is satisfied automatically; it serves as a check on the computation. The derivation is tedious, and we present only the results in second order,

\[ \hat{\eta}_1 = D_0 (u^2 / 3 - 1/2) e^{-\beta U(x)} \partial_x^2 e^{\beta U(x)}, \]

\[ \hat{\omega}_2 = D_0 (u^2 - 1/2) \left( \left( 4 \beta U''(x) \partial_x + 3 \beta U'''(x) \right) \partial_x e^{\beta U(x)} \right) + \left( u^2 - 1 \right) \left( 4 \beta U''(x) \partial_x + 3 \beta U'''(x) \right) \partial_x e^{\beta U(x)}, \]

\[ \hat{Z}_2 = D_0 (u^2 - 1/2) \beta U''(x) \left( 4 \beta U''(x) \right) \partial_x e^{\beta U(x)} + 3 \beta U'''(x) \partial_x. \] (4.23)

Again, the formulas (3.19) for \( U(x) = 0 \) are recovered. There are no contributions to \( \hat{Z}_n \) in this case, too, as expected according to the analysis in the previous Section. Also, linear potentials, \( U(x) = -Fx \), have no effect on validity of the uncorrected Smoluchowski equation (1.3).

The particle driven by a constant force \( F \) move asymptotically with constant mean velocity \( v_0 = F/\gamma \) and the distribution \( p(y, t) \) in coordinate \( y \), shifted by the drift, \( y = x - v_0 t \), is again Gaussian as in the case of no potential.

The situation becomes different if the driving force \( F(x) \) is not constant. If the mass \( m \) or the time of the thermalization \( t_0 = m/\gamma \) is small, but nonzero, the particle appearing at a new position \( x \) has to accommodate to the new local mean velocity. On the other hand, it carries some mean momentum from its previous position and needs some time to change it. Meanwhile it slips to some other position than predicted by purely stochastic dynamics due to its inertia, or non-zero mass. The effects of such slipping are indicated by the corrections \( \hat{Z}_n \).
of the Smoluchowski equation and they are nonzero for potentials with nonzero $U''(x)$, or higher derivatives.

As seen from Eq. (1.22), the $\tilde{Z}_n$ are not only functions, but operators, containing $\partial_x$ in the higher orders. So the mapped equation (4.19) has exactly the same structure as the mapped equations for diffusion [15], or biased diffusion [16, 22]. Being inspired by these works, Eq. (4.29) can be simplified by replacing the correction operators $D_0[1 + \sum_{k=1}^\infty t_k \tilde{Z}_k]$ by a function $D(x)$, a spatially dependent effective diffusion coefficient,

$$\partial_t p(x,t) = \partial_x e^{-\beta U(x)} D(x) \partial_x e^{\beta U(x)} p(x,t),$$

which becomes valid in the limit of stationary flow, i.e. when the spatial density $p$ and the flux $j$ change very slowly, $p(x,t) \to p(x)$. Due to mass conservation, Eq. (2.3), the flux $j(x,t) = j$ is constant (but nonzero) in $x$ as well. If expressed from Eq. (4.21),

$$j = -e^{-\beta U(x)} D(x) \partial_x e^{\beta U(x)} p(x),$$

the function $\partial_x (\exp[\beta U(x)] p(x)) = -j \exp[\beta U(x)]/D(x)$ is dependent only on the system; $m$, $\gamma$ and the potential $U(x)$, for any stationary solution $p(x)$. So we can substitute for it in Eq. (1.8),

$$j = D_0 e^{-\beta U(x)} \left[ 1 + \sum_{k=1}^{\infty} t_k \tilde{Z}_k(x) \right] e^{\beta U(x)} \frac{j}{D(x)},$$

(4.26) 

valid for stationary flow, and calculate $D(x)$ unambiguously from the expansion of the corrections $\tilde{Z}_k$.

$$\frac{D_0}{D(x)} = e^{-\beta U(x)} \left[ 1 + \sum_{k=1}^{\infty} t_k \tilde{Z}_k(x) \right]^{-1} e^{\beta U(x)},$$

(4.27)

as a series in $t_0$,

$$D(x)/D_0 = 1 + D_0 t_0 \beta U'' + (D_0 t_0)^2 \left[ 2 (\beta U'')^2 + \beta^2 U'' U(3) + \beta U''(4)/2 \right] + ...$$

(4.28)

The next simplification is that of neglecting all the derivatives but $U''(x)$, i.e. approximating the real $U(x)$ locally by a quadratic potential. In this case, the expansion (4.28) can be summed up to infinity,

$$D(x)/D_0 \approx \sum_{n=0}^{\infty} \frac{(2n)!}{n! (n+1)!} \left[ D_0 t_0 \beta U''(x) \right]^n = 1 - \sqrt{1 - 4D_0 t_0 \beta U''(x)}/2D_0 \beta U''(x),$$

(4.29)

the proof is given in the Appendix B. The formula works for $D_0 t_0 \beta U''(x) = mU''(x)/\gamma^2 < 1/4$, which is the condition for non-oscillatory movement of a particle in a quadratic well with friction, the damped harmonic oscillator. If $U''(x) = \kappa$ is constant, the trajectory of a particle averaged over the stochastic force is governed by

$$m \langle \dot{x} \rangle + \gamma \langle \dot{x} \rangle + \kappa \langle x \rangle = 0$$

(4.30)

from Eq. (1.1). The particular solutions are $\langle x(t) \rangle = \exp(\alpha t)$ with $\alpha = -(\gamma \pm \sqrt{\gamma^2 - 4m\kappa})/2m$. Requiring $\alpha$ to be a real number gives the same condition.

This simple example demonstrates restriction of the theory presented to non-oscillatory movement of the particle in potential wells on its way along a 1D channel. A small mass $m$ is expected, to enable the friction quickly damp the momentum of a particle; i.e. to have the relaxation in the velocity faster than in the real space coordinate $x$.

A more detailed insight to the restrictions of the dimensional reduction of the phase space controlled by the mass $m$ can be obtained by comparison of the Green’s function (GF) of the mapped equation (4.24) with $D(x)$ given by Eq. (4.29) and GF of the Kramers equation (1.2) for the damped harmonic oscillator, $U(x) = m x^2/2 = m \omega_0^2 x^2/2$, which is exactly solvable. The solution $G = G(x, v; t; x', v', t')$ of the equation

$$\left( \partial_t + v \partial_x - \omega_0^2 x \partial_v - \frac{\gamma}{\beta m^2} \partial_v e^{-\beta m v^2/2} \partial_v e^{\beta m v^2/2} \right) G$$

$$= \delta(x-x')\delta(v-v')\delta(t-t')$$

(4.31)

reads

$$G = \frac{(s_1 - s_2)e^{\gamma t/m}}{2\pi \sqrt{ab - h^2}} \exp \left[ - \left( a(\xi - \xi_0)^2 + b(\eta - \eta_0)^2 \right) + 2h(\xi - \xi_0)(\eta - \eta_0)/(2(ab - h^2)) \right],$$

(4.32)

where

$$s_1,2 = -\frac{\gamma}{2m} \pm \sqrt{\frac{\gamma^2}{4m^2} - \omega_0^2},$$

(4.33)

$$\xi = (s_1 x - v)e^{-s_2 t}, \quad \eta = (s_2 x - v)e^{-s_1 t},$$

$$\xi_0 = (s_1 x' - v'), \quad \eta_0 = (s_2 x' - v'),$$

$$a = \frac{\gamma}{\beta m s_1} \left( 1 - e^{-2s_1 t} \right), \quad b = \frac{\gamma}{\beta m s_2} \left( 1 - e^{-2s_2 t} \right),$$

$$h = \frac{2}{\beta m} \left( 1 - e^{-nt/m} \right).$$

(4.34)
Similar to the case of no potential in the Section III, let us suppose that a thermalized particle (equilibrated in velocity) was inserted at a position \( x_0 \) at time \( t' = 0 \),

\[
\rho_0(x',v') = \sqrt{\frac{\beta m}{2\pi}} \delta(x' - x_0)e^{-\beta mv'^2/2}.
\]  

(4.35)

After integration over \( v' \) and \( v \), we get the corresponding spatial density

\[
p(x,t) = \int_{-\infty}^{\infty} G(x,v,t;x',0)\rho_0(x',v')dx'dv = \\
\sqrt{\frac{\beta m}{2\pi}} \omega_0(s_1 - s_2) \exp \left[ -\frac{\beta m\omega_0^2}{2Z} \right] \\
\times \left( s_1(x - x_0e^{s_1t}) - s_2(x - x_0e^{s_2t}) \right)^2; \quad (4.36)
\]

\( Z = \left[ s_1(1 + e^{s_1t}) - s_2(1 + e^{s_1t}) \right] \left[ s_1(1 - e^{s_1t}) - s_2(1 - e^{s_1t}) \right] .
\]

On the other hand, the coefficient \( D(x) \), Eq. (4.29), becomes constant for the quadratic potential,

\[
D(x) = \frac{\gamma}{2m} - \sqrt{\frac{\gamma^2/4m^2 - \omega_0^2}{\beta m\omega_0^2}} = -\frac{s_1}{\beta m\omega_0^2}, \quad (4.37)
\]

and GF of the corresponding mapped equation (4.24),

\[
\left( \partial_t - \partial_x D(x)e^{-\beta m\omega_0^2/2} \partial_x e^{\beta m\omega_0^2x^2/2} \right) g(x,t;0,0) \\
= \delta(x - x_0)\delta(t - t_0), \quad (4.38)
\]

can be easily found by a calculation similar to the derivation of Eq. (3.1), Appendix A. The result,

\[
g(x,t;0,0) = \sqrt{\frac{\beta m}{2\pi}} \frac{1}{(1 - e^{2s_1t})} \omega_0 \exp \left[ -\frac{1}{2} \beta m\omega_0^2 \right] \\
\times \left( x - x_0e^{s_1t} \right)^2 \frac{1}{(1 - e^{2s_1t})}, \quad (4.39)
\]

describes evolution of the real space density of a thermalized particle inserted at \( x_0 \), too, and can be directly compared with the formula (4.36).

First, let us notice that in comparison with Eq. (4.36), the exponential \( e^{s_2t} \) disappeared from the formula (4.39). The root \( s_2 \simeq -\gamma/m \) for \( m \to 0 \) makes \( e^{s_2t} \simeq e^{-\gamma t/m} \) the term essentially singular in \( m \) and so invisible for the recurrence procedure, which works with the operators \( \hat{\omega} \) and \( \hat{\eta} \) expanded in \( m \). Using our argumentation from the Section III, \( e^{s_1t} \) represents the "transients" neglected by the mapping. On the other hand, \( e^{s_1t} \simeq e^{-m\omega_0^2t/\gamma} \) is regular in \( m \) small, representing the contribution of the low-lying states, retained by the method.

Next, let us stress that the equation (4.24) with \( D(x) \) expressed by the expansion (4.28) was derived in the limit of the stationary flow; for the net flux almost constant, which is not the case of the process described by the Eqs. (4.36) and (4.39). Nevertheless, using the approximations

\[
s_1 - s_2(1 \pm e^{s_1t}) \simeq (s_1 - s_2)(1 \pm e^{s_1t}),
\]

\[
s_1x - s_2(x - x_0e^{s_1t}) \simeq (s_1 - s_2)(x - x_0e^{s_1t}),
\]

applicable for \( e^{s_1t} \ll 1 \), the regularized formula (4.36) (with \( e^{s_2t} \) neglected) becomes finally Eq. (4.39); i.e. it represents correctly the asymptotic behavior of the spatial density \( p(x,t) \) for large time \( t \).

If \( m \) approaches \( \gamma/2\omega_0 \), the transients contributing by \( e^{s_2t} \), neglected by the mapping, become important. In the oscillating regime, \( s_{1,2} \) are complex numbers and both are necessary for expressing the real density \( p(x,t) \) in Eq. (4.39). The mapping which splits the Hilbert space into the retained low-lying states and the neglected transients, controlled by \( m \) small, loses its justification and the method stops working. Mapping in this region requires a different method to be applied. It will be an object of our study in the future.

V. CONCLUSION

Although modeling of transport in confined systems is often based on study of the Langevin equation, Eq. (1.1) in the simplest 1D case, the solutions necessary in practical applications are often accessible only in two limits: either the friction \( \gamma \to 0 \), when the particles obey Newtonian dynamics, or the mass \( m \to 0 \), which corresponds to stochastic dynamics. Any solution in the region between these limits requires working in phase space, which makes the problem much more complicated.

The present paper shows how to describe the region of finite \( m/\gamma \) while still working in real space, as in the case of stochastic dynamics. The equation governing evolution of the spatial density \( p(x,t) \) is the Smoluchowski equation, corresponding to the limit of a massless particle, extended by a series of corrections in powers of \( t_0 = m/\gamma \); \( t_0 \) can be interpreted as the typical time of thermalizing of the particle’s initial velocity by the stochastic force.

In general, the extended Smoluchowski equation has the form of Eq. (1.1), \( D_0 = 1/\gamma \beta \) denotes the diffusion constant and the operators \( \hat{Z}_k \) are systematically derived within the recurrence procedure presented in the Sect. IV. In the limit of stationary flow, i.e. when the flux is almost constant but nonzero in time and space, this equation can be simplified to Eq. (4.24), where the effective diffusion coefficient \( D(x) \) is calculated unambiguously from the operators \( \hat{Z}_k \), Eq. (4.25). In the simplest approximation, when all the derivatives of the potential higher than \( U''(x) \) are neglected, the series of corrections can be summed up to infinity, giving the formula for \( D(x) \) in a closed form, Eq. (4.29), described in Fig. 1. Then the equation describes stationary flow in a quadratic potential. The theory works while \( 4mU''(x) < \gamma^2 \), until the
averaged trajectory of a single particle is not oscillatory in the potential wells along the 1D channel. The mapping in the oscillatory regime requires the next analysis, which will be done in the future.

Technically, the paper demonstrates that the projection technique developed for mapping of diffusion in 2D (3D) channels with varying cross section [13, 14, 16], can be adapted for the dimensional reduction of a process described by an evolution equation of a different type than the diffusion or Smoluchowski equation. The method has been modified significantly; $m/\gamma$ had to be confirmed as the small parameter controlling the expansion of the corrections $\tilde{Z}_k$, as well as the operators of the backward mapping, $\tilde{w}$ and $\tilde{\eta}$. In contrast to diffusion, the flux $D(x,t)$ is handled here as a quantity independent of the density $p(x,t)$. Thus the recurrence procedure, calculating expansions of the correction operators $\tilde{Z}_k$ and the operators $\tilde{w}$, $\tilde{\eta}$, is in principle the result of combination of three equations, Eqs. (1.2), (2.3) and also (2.5), with the relation of the backward mapping, Eq. (2.9).

It is worthwhile to notice that including the mass dependent corrections to the Smoluchowski equation results in the equations (4.9) or (4.24), which of the same form as the comparable equations obtained from the mapping of diffusion in channels with varying cross section. On the other hand, the effective coefficient $D(x)$ has a different symmetry than the similar formulas extending the Fick-Jacobs equation [16, 17] for confined diffusion. Also $D(x)$ can be greater than 1 here (see Fig. 1); i.e. the quasi stationary flux is accelerated when passing through a shallow potential well, depending on the nonzero mass of the particles. These interesting properties could be observed in simulations similar to that verifying $D(x)$ in the extended Fick-Jacobs equation [27, 28]. The effects of slipping of the particles diffusing under a nonconstant force $F(x)$ due to their inertia, as described in Sect. IV, might also influence the interesting phenomena in the micro and nano world, such as Brownian pumps [29, 30], rectification of the flux in quasi 1D structures [31], stochastic resonance [20, 32, 34], or the negative mobility [35]. Study of such applications of the theory presented is expected in the future.

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APPENDIX A: EXACT SOLUTION

The Green’s function solving the FP equation with zero potential, Eq. (3.1), is calculated here. First we introduce the scaled coordinates $\xi, u, \tau$ according to Eqs. (3.3) and define the function $\Gamma(\xi, u, \tau; \xi', u', \tau')$,

$$G(x,v,t;x',v',t') = e^{-u'^2/2}\Gamma(\xi, u, \tau; \xi', u', \tau')e^{u^2/2},$$

(A1)

satisfying the transformed equation (A1).

$$\left[ \partial_\tau + u \partial_\xi - \partial_u^2 + u^2 - 1 \right] \Gamma(\xi, u, \tau; \xi', u', \tau') = \frac{\gamma \beta}{4} e^{(u'^2-u^2)/2}\delta(\xi - \xi')\delta(u - u')\delta(\tau - \tau').$$

(A2)

the exponential factor becomes unity due to $\delta(u - u')$.

After the Fourier transform in $\xi$ and $\tau$,

$$\Gamma(\xi, u, \tau; \xi', u', \tau') = \int \frac{dkd\nu}{4\pi^2} e^{ik(\xi - \xi') - \nu(\tau - \tau')} \Gamma_{k,\nu}(u; u'),$$

(A3)

and shifting the velocities by $ik/2$, $w = u + ik/2$ and $w' = u' + ik/2$, the equation

$$[-i\nu - \partial_w^2 + u^2 - 1 + k^2/4] \Gamma_{k,\nu}(w; w') = \frac{\gamma \beta}{4} \delta(u - u')$$

(A4)

becomes solvable if $\Gamma_{k,\nu}(w; w')$ is expressed in the basis set of the linear harmonic oscillator $\psi_n(w)$,

$$\Gamma_{k,\nu}(w; w') = \sum_{n=0}^{\infty} \Gamma_n(k, \nu)\psi_n(w)\psi_n^*(w').$$

(A5)

The eigenfunctions $\psi_n(w)$ satisfy

$$(-\partial_w^2 + w^2) \psi_n(w) = \lambda_n \psi_n(w) = (2n + 1) \psi_n(w)$$

(A6)

and we use the integral representation of the Hermite polynomials $H_n(w)$

$$\psi_n(w) = \frac{1}{\sqrt{\pi} \sqrt{2^n n!}} H_n(w)e^{-w^2/2}$$

$$= \sqrt{\frac{2^n}{n!\pi^{3/2}}} e^{-w^2/2} \int_{-\infty}^{\infty} (w + iv)^n e^{-r^2} dr$$

(A7)

in the next calculation.

Using the transformations above, we find

$$\Gamma_n(k, \nu) = \frac{\gamma \beta}{4(\nu - \lambda_n + 1 + k^2/4)}.$$ 

(A8)

Applying it in the formulas (A5) and (A3), we integrate the last one over $\nu$ in the complex plane,

$$\Gamma(\xi, u, \tau; \xi', u', \tau') = \frac{\Theta(\tau - \tau')} {8\pi D_0} \int_{-\infty}^{\infty} e^{ik(\xi - \xi') - k^2(\tau - \tau'}/4$$

$$\times \sum_{n=0}^{\infty} e^{-2n(\tau - \tau')} \psi_n(w)\psi_n^*(w'),$$

(A9)

$\Theta(x)$ denotes the Heaviside step function and $D_0 = 1/\gamma \beta$ is the diffusion constant. Now the integral relation (A7) is used for $\psi_n(w)$ and $\psi_n^*(w')$ and the summation over $n$ can be readily completed. Finally, the straightforward triple integration over $k$, $\tau$, $\tau'$ is performed and using the transformation (A1) results in the formula (3.2).
APPENDIX B: QUADRATIC APPROXIMATION

Derivation of the formula (1.24) for the effective diffusion coefficient $D(x)$ with all the derivatives higher than $U''(x)$ neglected is presented here. This approximation corresponds to local replacing of the potential by a parabola, $U(x) \simeq \kappa (x - x_0)^2/2 + U_0$, where $\kappa$, $x_0$ and $U_0$ are fitting parameters.

First we simplify Eq. (1.27). For quadratic potential, the right hand side can be rewritten as

$$e^{-\beta U(x)} \left(1 + t_0 \hat{Z} \right)^{-1} e^{\beta U(x)} = \left(1 + t_0 e^{-\beta U \hat{Z}(x) e^{\beta U}} \right)^{-1},$$

$$t_0 \hat{Z} = \sum_{n=1}^{\infty} t_0 \hat{Z}_n; \text{ the difference contains only the higher derivatives of } U(x), \text{ which are zero. Hence}$$

$$D(x)/D_0 = 1 + e^{-\beta U(x)} \sum_{n=1}^{\infty} t_0^n \hat{Z}_n e^{\beta U(x)}. \quad \text{(B1)}$$

The formulas for $D(x)$ have been derived considering stationary flow: $j(x, t) = j$ is constant. It simplifies the relation (1.7); $\partial_x j = 0$. Thus the right hand side represents stationary flux, which can be directly compared with Eq. (1.8), giving a much simpler relation between $\hat{Z}_n$ and $\hat{I}_n$ than Eq. (1.10),

$$e^{-\beta U(x)} \hat{Z}_n(x) \partial_x e^{\beta U(x)} p(x) = \partial_x \hat{I}_n(x) p(x) \quad \text{(B2)}$$

for any stationary solution $p(x)$. Calculation of the coefficients of $D(x)$ according to Eq. (1.9) requires us to take $\partial_x \exp[\beta U(x)] p(x) = \exp[\beta U(x)]$, hence finally

$$e^{-\beta U(x)} \hat{Z}_n e^{\beta U(x)} = \frac{2}{\sqrt{\pi}} \partial_x \int_{-\infty}^{\infty} u^2 e^{-u^2} \times \hat{\omega}_n(x, u) e^{-\beta U(x)} \int dx e^{\beta U(x)} \quad \text{(B3)}$$

after application of Eq. (1.6).

Before writing the explicit formulas for $\hat{\omega}_n$ for the quadratic potential, we define the polynomials

$$P_n(u) = \sum_{k=0}^{n} \frac{(-1)^{n-k} 2k^n}{(2k)![(n-k)!]^2} u^{2k},$$

$$Q_n(u) = \sum_{k=0}^{n} \frac{(-1)^{n-k} 2k^{n-k}}{(2k+1)!(n-k)!} u^{2k}, \quad \text{(B4)}$$

$n = 1, 2, ..., \text{ coming from the expansions of } \hat{\omega}_n \text{ and } \hat{\eta}_n \text{ for zero potential in } t_0, \text{ Eqs. (3.19). The first few polynomials are visible in the round brackets of Eq. (3.19). One can check by direct integration that}$

$$\int_{-\infty}^{\infty} Q_n(u) u^2 e^{-u^2} du = \frac{\sqrt{\pi}}{2^{n+1}} \sum_{k=0}^{n} \frac{(-1)^{n-k}}{k!(n-k)!} = 0,$$

$$\int_{-\infty}^{\infty} P_n(u) u^2 e^{-u^2} du = \frac{\sqrt{\pi}}{2} \delta_{n,1}, \quad \text{(B5)}$$

corresponding to the normalization of $\hat{\eta}_n$, Eq. (4.5), and the relations (3.10), (3.17), proving no correction to the Smoluchowski equation in the case $U(x) = 0$.

The operators $\hat{\omega}_n$ and $\hat{\eta}_n$ for the quadratic potential have the form

$$\hat{\omega}_n = e^{-\beta U(x)} \sum_{k=1}^{n} c_{n,k} P_k(u) (\beta U'')^{-n-k} \partial_x^{2k} e^{\beta U(x)},$$

$$\hat{\eta}_n = e^{-\beta U(x)} \sum_{k=1}^{n} c_{n,k} B_k(u) (\beta U'')^{-n-k} \partial_x^{2k} e^{\beta U(x)}, \quad \text{(B6)}$$

with the coefficients

$$c_{n,k} = D_0^n \frac{2k (2n-1)!}{(n-k)!(n+k)!} \quad \text{(B7)}$$

due to the integrals, Eq. (B5), only the first terms with $P_1(u)$ in Eq. (B6) contribute to the expansion of $D(x)$, Eq. (1.5). Then the functions become

$$e^{-\beta U(x)} \hat{Z}_n e^{\beta U(x)} = c_{n,1} \partial_x e^{-\beta U(x)} (\beta U'')^{-n-1} \partial_x e^{\beta U(x)}$$

$$= \frac{2}{(n-1)! (n+1)!} (D_0 \beta U''^n), \quad \text{(B8)}$$

taking $U^{(3)}(x) = 0$ into account. Applied in Eq. (1.9) it results in the expansion of $D(x)$, Eq. (1.29).

Finally, one has to verify that the formulas (B6) satisfy the recurrence relations (4.13) and (4.17), acting on the function $p(x) = \exp[-\beta U(x)] \int dx \exp[\beta U(x)]$. Although the equations simplify notably due to neglecting the derivatives higher than $U''(x)$, we omit the details of this tedious but straightforward calculation.

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