Classical diffusion in channels with a spatially varying cross-section

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We study the diffusion of classical particles in channels with varying boundaries. The problem is characterized by the Neumann boundary condition (zero normal current) in contrast to the Dirichlet boundary condition (zero function) for ''quantum confinement'' problems. Eliminating transverse modes, we derive an effective diffusion equation that describes particle propagation in the space of reduced dimension in the presence of a frozen drift field. The latter stems from boundary variations of the original boundary problem. Boundary variations may thus result in an appreciable change of the particle transport and, in particular, in a nonlinear response to an external field. We show also that there is a difference between the nonlinear responses of open and closed channels.

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I. INTRODUCTION

Diffusion of classical particles in a spatially random time-independent velocity field continue to attract interest. Early studies (see [1–4] and references therein) have revealed various anomalous diffusion regimes that may take place for a long-range correlated velocity field. It has been also shown [4] that the considered classical model possesses nonselfaveraging effects, which bear resemblance to mesoscopic effects of (quantum) weak localization [5]. Recently this classical model has attracted renewed attention, motivated, in particular, by the interest in properties of random non-Hermitian operators [6], chemical reactions in disordered media [7], etc.

In contrast to previous studies of classical diffusion in random but unbounded media, here we consider a different physical situation, namely, the classical diffusion in a channel (slab, pipe, wire, etc.) with time-independent spatial variations of the channel boundary. We are looking for classical analogies to (and differences with) confinement effects known for ''quantum'' particles. In the latter case these effects are due to spatial variations of the energy of the particle tranverse motion (confinement energy). These variations result in the appearance of a random potential in an effective (Schrödinger) equation for the particle propagation along the channel (in a space of reduced dimension). Of course, this phenomenon is not restricted to quantum particles but is common for any wave obeying the Dirichlet boundary condition (zero amplitude). On the contrary, the classical diffusion is characterized by the Neumann condition (zero normal current) at the channel boundary. We show that this leads to quite a different form of an effective equation for the motion along the channel: there appears a space-dependent field of frozen drift forces (velocities). Thus, the original boundary problem [see Eqs.(1) and (2) below] is mapped on the abovementioned problem Eq. (23) of classical diffusion in unbounded media in the presence of a frozen random velocity field [Eqs. (24) or (36)]. The arising velocity field corresponds to potential fIows, which is the consequence of the Hermitian nature of the original boundary problem. Therefore, long-range correlated variations of the channel boundary may result in a subdiffusion regime in accordance with earlier findings for the unbounded diffusion in the presence of random potential flows [2–4]. Furthermore, we consider another interesting feature of classical diffusion in channels with spatially varying boundaries: a nonlinearity of the response to an external force, that occurs even for field independent bare values of kinetic parameters and that is absent for channels with a constant cross section. We also demonstrate that there is a remarkable difference in nonlinear responses of open Eq. (42) and closed Eq. (47) channels to an external force applied along the channel. This difference (vanishing in the linear regime) bears resemblance to a difference in some physical properties of open and closed mesoscopic samples [8,9].

This paper has the following structure. In Sec. II we perform a transformation of coordinates that maps the original problem with the varying boundary to a problem with flat boundary but with modified boundary conditions. We derive equations for transverse harmonics of the Green's function of the transformed equation, using a weak coupling between the zero and nonzero harmonics. In Sec. III we consider small variations of the boundary; eliminating the nonzero harmonics we obtain an effective diffusion equation for the long-scale limit of the original problem. This equation contains a frozen drift field as well as a spatial modulation of the diffusion coefficient. In Sec. IV we consider the case of random drifts (random variations of the channel boundary) and calculate corrections to the effective diffusion coefficient for disorder averaged propagation. In Sec. V an effective diffusion equation is derived for the case of nonsmall but smooth variations of the channel boundary. In Sec. VI we discuss in more detail the particular case of stationary diffusion through an effectively one-dimensional channel under the action of an external force. The nonlinear current response is calculated for open and closed channels with smoothly varying boundaries. In conclusion we summarize and discuss the obtained results.

II. BASIC EQUATIONS

A. Formulation of the problem

First we consider a channel in the form of a film of average thickness L_z with the upper and lower boundaries $z=f_u(\mathbf{r})$ and $z=f_l(\mathbf{r})$ ($f_l<f_u$); $\mathbf{r}$ is a radius vector in the d-dimensional ($d=2$ for a film or $d=1$ for a surface channel) subspace orthogonal to the z axis. Later in the paper we shall consider also channels with more complicated boundaries.

The Green's function of the diffusion equation in the film obeys the equation

$$[-i\omega-D\boldsymbol{\nabla}^2]G(\boldsymbol{r},\boldsymbol{z};\boldsymbol{r}',\boldsymbol{z}')=\delta(\boldsymbol{z}-\boldsymbol{z}')\,\delta(\boldsymbol{r}-\boldsymbol{r}') \tag{1}$$

and the Neumann boundary condition (zero normal current)

$$(\mathbf{n}\cdot\boldsymbol{\nabla})G(\boldsymbol{r},\boldsymbol{z};\boldsymbol{r}',\boldsymbol{z}')|_{\mathbf{r}\in B}=0 \tag{2}$$

on the film boundary B. In Eqs. (1) and (2) D is the bare diffusion coefficient; $\boldsymbol{\nabla}=(\partial/\partial r_\alpha,\partial/\partial z)$, $\alpha=1,\ \ldots,\ d$; and $\mathbf{n}$ is the normal vector to the boundary surface: $\mathbf{n}\propto[-\partial f(\mathbf{r})/\partial r_\alpha,1]$. We are interested in small frequency ($\omega\ll D/L_z^2$), long-distance ($|\mathbf{r}-\mathbf{r}'|\gg L_z$) properties of the diffusion propagator; our task is to obtain an effective equation for a reduced function

$$G(\boldsymbol{r},\boldsymbol{r}')=\int_{f_l(\boldsymbol{r})}^{f_u(\boldsymbol{r})}dz\int_{f_l(\boldsymbol{r}')}^{f_u(\boldsymbol{r}')}dz'\frac{G(\boldsymbol{r},\boldsymbol{z};\boldsymbol{r}',\boldsymbol{z}')}{f_u(\boldsymbol{r}')-f_l(\boldsymbol{r}')}, \tag{3}$$

which describes macroscopic transport along the channel (in the space of the reduced dimension d) from a source located at a point $\mathbf{r}'$. In the definition (3), integration over z' (with a weight $[f_u(\mathbf{r}')-f_l(\mathbf{r}')]^{-1}$) corresponds to a source of unit power spread uniformly along the z direction of the film, rather than to a source concentrated at some point $z'=z_0$. However, the difference between the two variants vanishes in the macroscopic limit of interest.

B. Derivation of basic equations

In the analysis of the problem formulated in Eqs. (1) and (2), it is convenient to use a trick known in the theory of light scattering from rough surfaces, namely, to perform a coordinate transformation that makes the boundaries flat. To simplify the following expressions, below we restrict the derivation to the simpler case where only the upper boundary varies, while the lower one is flat ($f_l=0$). In this case, we use new coordinates:

$$\rho_\alpha=r_\alpha;\qquad \eta=zL_z/f_u(\mathbf{r}), \tag{4}$$

(the lower index "u" will be omitted below) which make the boundary B flat ($B=B_++B_-$; $B_+:\ \eta=L_z$; $B_-:\ \eta=0$). Equation (4) induces the transformation of derivatives:

$$\partial/\partial r_\alpha=\partial_\alpha-(\partial_\alpha\ln f)\,\eta\partial/\partial\eta;\qquad \partial/\partial z=(L_z/f)\partial/\partial\eta, \tag{5}$$

where $\partial_\alpha\equiv\partial/\partial\rho_\alpha$. In the new coordinates, Eq. (1) for

$$\mathcal{G}(\boldsymbol{\rho},\eta;\boldsymbol{\rho}',\eta')=G(\boldsymbol{r},\boldsymbol{z};\boldsymbol{r}',\boldsymbol{z}') \tag{6}$$

takes the form

$$[-i\omega-D(\partial_\alpha^2+\partial^2/\partial\eta^2+\hat{U}(\boldsymbol{\rho},\eta))]\mathcal{G}(\boldsymbol{\rho},\eta;\boldsymbol{\rho}',\eta')=\delta(\boldsymbol{\rho}-\boldsymbol{\rho}')\,\delta(\eta-\eta')L_z/f(\boldsymbol{\rho}'), \tag{7}$$

where the factor $L_z/f(\boldsymbol{\rho}')$ on the right-hand side stems from the Jacobian of the transformation (4), and the operator $\hat{U}$ is

$$\hat{U}(\boldsymbol{\rho},\eta)=-[2(\partial_\alpha\ln f)\partial_\alpha+(\partial_\alpha^2\ln f)]\,\eta\partial/\partial\eta+(\partial_\alpha\ln f)^2(\eta\partial/\partial\eta)^2+[L_z^2/f^2-1]\partial^2/\partial\eta^2. \tag{8}$$

A generalization of Eq. (4) for two varying boundaries is straightforward: $\eta=L_z(z-f_l)/(f_u-f_l)$. In an equivalent form it has been used recently [10] for studying transport processes in rough films, with the boundary roughness treated as the reason of the momentum relaxation of particles (waves) propagating ballistically in the bulk of the film. A set of physical problems considered in [10] corresponds to the Dirichlet boundary condition (vanishing amplitude: $\Psi|_B=0$) that remains invariant under the coordinate transformation. On the contrary, for the diffusive motion considered in the present paper, we face a more complicated situation as the Neumann boundary condition (2) is affected by the transformation and takes the form

$$[\partial/\partial\eta-\hat{V}_\eta(\boldsymbol{\rho})]\mathcal{G}(\boldsymbol{\rho},\eta;\ \boldsymbol{\rho}',\eta')=0\quad\text{at } \eta=0,\ L_z. \tag{9}$$

Here

$$\hat{V}_0=0;\qquad \hat{V}_{L_z}=\frac{f\partial_\alpha f}{L_z[1+(\partial_\alpha f)^2]}\partial_\alpha. \tag{10}$$

Thus, the original problem is reformulated now for the flat boundaries but with perturbation terms both in Eq. (7) and in the boundary condition Eq. (9). To develop a regular perturbative treatment, we introduce a Green's function $\mathcal{G}^{(0)}(\boldsymbol{\rho}-\boldsymbol{\rho}';\eta,\eta')$ of an unperturbed problem. This function is determined by the equation

$$[-i\omega-D\boldsymbol{\nabla}_\xi^2]\mathcal{G}^{(0)}(\boldsymbol{\rho}-\boldsymbol{\rho}';\eta,\eta')=\delta(\boldsymbol{\xi}-\boldsymbol{\xi}'), \tag{11}$$

(where shortened notations $\boldsymbol{\xi}=(\boldsymbol{\rho},\eta)$ and $\boldsymbol{\nabla}_\xi^2\equiv\partial_\alpha^2+\partial^2/\partial\eta^2$ are introduced) and by the Neumann boundary condition at the flat boundaries

$$\partial/\partial\eta\,\mathcal{G}^{(0)}(\boldsymbol{\rho}-\boldsymbol{\rho}';\eta,\eta')=0\quad\text{at } \eta=0,\ L_z. \tag{12}$$

Following the usual method (see, e.g., Ref. [11]) we multiply Eq. (7) by $\mathcal{G}^{(0)}$ and Eq. (11) by $\mathcal{G}$, and integrate their difference. With the use of Green's theorem and the boundary conditions (9) and (12), we arrive at the following integral equation for $\mathcal{G}$:

$$\mathcal{G}(\boldsymbol{\xi};\boldsymbol{\xi}')=\mathcal{G}^{(0)}(\boldsymbol{\rho}-\boldsymbol{\rho}';\eta,\eta')L_z/f(\boldsymbol{\rho}')+D\int d\boldsymbol{\rho}_1[\mathcal{G}^{(0)}(\boldsymbol{\rho}-\boldsymbol{\rho}_1;\eta,\eta_1)\hat{V}_{\eta_1}(\boldsymbol{\rho}_1)\times\mathcal{G}(\boldsymbol{\xi}_1;\boldsymbol{\xi}')]_{\eta_1=0}^{\eta_1=L_z}+D\int d\boldsymbol{\xi}_1\mathcal{G}^{(0)}(\boldsymbol{\rho}-\boldsymbol{\rho}_1;\eta,\eta_1)\times\hat{U}(\boldsymbol{\xi}_1)\mathcal{G}(\boldsymbol{\xi}_1;\boldsymbol{\xi}'). \tag{13}$$

Now we sketch main steps of the further evaluation. In the basis of eigenstates of the unperturbed problem, the function $\mathcal{G}^{(0)}(\boldsymbol{\rho}-\boldsymbol{\rho}';\eta,\eta')$ may be represented as

$$\mathcal{G}^{(0)}(\boldsymbol{\rho}-\boldsymbol{\rho}';\eta,\eta')=\frac{1}{L_z}\mathcal{G}_0^{(0)}(\boldsymbol{\rho}-\boldsymbol{\rho}')+\frac{2}{L_z}\sum_{n>0}\mathcal{G}_n^{(0)}(\boldsymbol{\rho}-\boldsymbol{\rho}')\times\cos\left(\frac{\pi n\eta}{L_z}\right)\cos\left(\frac{\pi n\eta'}{L_z}\right), \tag{14}$$

where the Fourier transform of the functions $\mathcal{G}_n^{(0)}(\boldsymbol{\rho})$ is

$$\mathcal{G}_n^{(0)}(\boldsymbol{q})=[-i\omega+Dq^2+D\pi^2n^2/L_z^2]^{-1}. \tag{15}$$

Integrating Eq. (13) over η' we obtain an equation for the function

$$\mathcal{G}(\boldsymbol{\rho},\boldsymbol{\rho}';\eta)=\int_0^{L_z}\mathcal{G}(\boldsymbol{\rho},\eta;\boldsymbol{\rho}'\,\eta')d\eta'/L_z. \tag{16}$$

The equation for $\mathcal{G}(\boldsymbol{\rho},\boldsymbol{\rho}';\eta)$ derived in this way differs from Eq. (13) only by the first term on the rhs: the function $\mathcal{G}^{(0)}(\boldsymbol{\rho}-\boldsymbol{\rho}';\eta,\eta')$ is replaced by its zero transverse harmonic $\mathcal{G}_0^{(0)}(\boldsymbol{\rho}-\boldsymbol{\rho}')$. Looking for $\mathcal{G}(\boldsymbol{\rho},\boldsymbol{\rho}';\eta)$ in the form

$$\mathcal{G}(\boldsymbol{\rho},\boldsymbol{\rho}';\eta)=\frac{1}{L_z}\mathcal{G}(\boldsymbol{\rho},\boldsymbol{\rho}')+\frac{2}{L_z}\sum_{n>0}\mathcal{G}_n(\boldsymbol{\rho},\boldsymbol{\rho}')\cos\left(\frac{\pi n\eta}{L_z}\right), \tag{17}$$

we obtain an infinite system of coupled equations for transverse harmonics $\mathcal{G}(\boldsymbol{\rho},\boldsymbol{\rho}')$ and $\mathcal{G}_n(\boldsymbol{\rho},\boldsymbol{\rho}')$. Note that because of the weak convergency of the series Eq. (17) near the boundary, one may not interchange the summation over n and differentiation with respect to η. Therefore, before applying Eq. (17), some care is needed with respect to terms of $\hat{U}$ that contain derivatives with respect to η: using integration by parts, the action of these (transverse) derivatives may be transferred to the unperturbed function $\mathcal{G}^{(0)}(\boldsymbol{\rho}-\boldsymbol{\rho}';\eta,\eta')$. Surface terms arising in the course of the integration by parts are added to those present already in Eq. (13). Due to the elimination of fast transverse derivatives, this integration by parts leads to a system of equations for $\mathcal{G}(\boldsymbol{\rho},\boldsymbol{\rho}')$ and $\mathcal{G}_n(\boldsymbol{\rho},\boldsymbol{\rho}')$, with improved convergence with respect to the perturbative exclusion of nonzero transverse harmonics $\mathcal{G}_n(\boldsymbol{\rho},\boldsymbol{\rho}')$ with $n>0$.

Here we apply this general routine to derive an effective equation for the zero transverse harmonic $\mathcal{G}(\boldsymbol{\rho},\boldsymbol{\rho}')$. This is possible if variations of the channel boundary are relatively small ($|\delta f|/f\ll 1$) or smooth on the scale of L_z ($L_z|\partial_\alpha f|\ll f$). The two conditions may be written as $|\partial_\alpha f|\ll 1$. Taking into account terms up to second order in the small quantity $|\partial_\alpha f|\ll 1$ we obtain the following equations for the transverse harmonics:

$$\left[-i\omega-D\partial_\alpha^2-\frac{DL_z}{f^2(\rho)}\hat{V}_{L_z}(\boldsymbol{\rho})\right]\mathcal{G}(\boldsymbol{\rho},\boldsymbol{\rho}')=\delta(\boldsymbol{\rho}-\boldsymbol{\rho}')\frac{L_z}{f(\boldsymbol{\rho})}+2D\left[\frac{L_z}{f^2(\boldsymbol{\rho})}\hat{V}_{L_z}(\boldsymbol{\rho})+\hat{U}_1(\boldsymbol{\rho})\right]\times\sum_{n>0}(-1)^n\mathcal{G}_n(\boldsymbol{\rho},\boldsymbol{\rho}'), \tag{18}$$

$$\left[-i\omega-D\partial_\alpha^2+D\frac{\pi^2n^2}{f^2(\rho)}\right]\mathcal{G}_n(\boldsymbol{\rho},\boldsymbol{\rho}')=(-1)^n\frac{DL_z}{f^2(\boldsymbol{\rho})}\hat{V}_{L_z}(\boldsymbol{\rho})\mathcal{G}(\boldsymbol{\rho},\boldsymbol{\rho}') \tag{19}$$

with $\hat{U}_1=-[2(\partial_\alpha\ln f)\partial_\alpha+(\partial_\alpha^2\ln f)]$.

In the following section we consider the case of small channel boundary variations. Later we shall also discuss the case of arbitrary but smooth boundary variations.

III. SMALL BOUNDARY VARIATIONS

A. Effective diffusion equation

To treat the case of small boundary variations we write the function $f(\boldsymbol{r})$, determining the channel (upper) boundary $z=f(\boldsymbol{r})$, in the form,

$$f(\boldsymbol{r})=L_z[1+h(\boldsymbol{r})], \tag{20}$$

with $h\ll 1$. The coupling of different transverse harmonics, $\mathcal{G}(\boldsymbol{\rho},\boldsymbol{\rho}')$ and $\mathcal{G}_n(\boldsymbol{\rho},\boldsymbol{\rho}')$ is determined by the small function $h(r)$. From Eq. (18) we find for $\mathcal{G}_n(\boldsymbol{\rho},\boldsymbol{\rho}')$:

$$\mathcal{G}_n(\boldsymbol{\rho},\boldsymbol{\rho}')=\frac{(-1)^nD}{L_z}\int d\boldsymbol{\rho}_1\mathcal{G}_n^{(0)}(\boldsymbol{\rho}-\boldsymbol{\rho}_1)\hat{V}_{L_z}(\boldsymbol{\rho}_1)\mathcal{G}(\boldsymbol{\rho},\boldsymbol{\rho}'), \tag{21}$$

valid in the first order in h. Using Eq. (19) to substitute nonzero harmonics $\mathcal{G}_n(\boldsymbol{\rho},\boldsymbol{\rho}')$, which enter Eq. (18), we find eventually a closed equation for $\mathcal{G}(\boldsymbol{\rho},\boldsymbol{\rho}')$ valid up to the second order in h. Comparing Eqs. (3), (16), and (17), we find that $\mathcal{G}(\boldsymbol{\rho},\boldsymbol{\rho}')$ differs only by a factor from the function of interest $G(\boldsymbol{r},\boldsymbol{r}')$:

$$\mathcal{G}(\boldsymbol{r},\boldsymbol{r}')=[L_z/f(\boldsymbol{r})]G(\boldsymbol{r},\boldsymbol{r}'). \tag{22}$$

This factor $L_z/f(\boldsymbol{r})$ stems from the Jacobian of the coordinate transformation. (Note, that after eliminating the transverse coordinate, we do not need to distinguish anymore between coordinates $\mathbf{r}$ and $\boldsymbol{\rho}$ in the longitudinal subspace of the reduced dimension d). Using Eq. (22) we arrive at the following equation for $G(\boldsymbol{r},\boldsymbol{r}')$:

$$\{-i\omega+\partial_\alpha[v_\alpha(\boldsymbol{r})-\hat{D}_{\alpha,\beta}\partial_\beta]\}G(\boldsymbol{r},\boldsymbol{r}')=\delta(\boldsymbol{r}-\boldsymbol{r}'). \tag{23}$$

In Eq. (23)

$$v_\alpha(\boldsymbol{r}) = D[1-h(\boldsymbol{r})]\partial_\alpha h(\boldsymbol{r}), \tag{24}$$

and the symbolic operator notation $\hat{D}_{\alpha,\beta}\partial_\beta \ldots$ means

$$[\hat{D}_{\alpha,\beta}\partial_\beta G](\boldsymbol{r},\boldsymbol{r}') = D\int d\boldsymbol{r}_1\{\delta_{\alpha,\beta}\delta(\boldsymbol{r}-\boldsymbol{r}_1) - DL_z[\partial_\alpha h(\boldsymbol{r})]F(\boldsymbol{r}-\boldsymbol{r}_1) \times[\partial_{1\beta}h(\boldsymbol{r}_1)]\}\partial_{1\beta}G(\boldsymbol{r}_1,\boldsymbol{r}'), \tag{25}$$

where the Fourier transform of the function $F(\boldsymbol{\rho})$ is given by

$$F(\boldsymbol{q}) = \frac{2}{L_z}\sum_{n>0}\frac{1}{[-i\omega+Dq^2+\pi^2 n^2 D/L_z^2]}. \tag{26}$$

The function $F(\boldsymbol{\rho}) = \mathcal{G}^{(0)}(\boldsymbol{\rho},0;0) - \mathcal{G}_0^{(0)}(\boldsymbol{\rho})$ decays fast at distances $\boldsymbol{\rho} > L_z$.

The effective diffusion equation (23) guarantees the particle conservation law. Equations (23)–(25) fulfill the program formulated in the Introduction: the complicated problem of diffusion in a $(d+1)$-dimensional channel of variable thickness is reduced to the simpler problem of diffusion in a uniform d-dimensional layer in the presence of a frozen field. The latter class of problems allows for a regular field-theoretical treatment. The frozen field (24) is a potential field, which corresponds to the model 3 of [2,4]. In the present section the reduction has been performed for the case of small boundary deviations, $|\mathbf{h}| \ll 1$.

Now we use Eqs. (23)–(25) to calculate a correction to the bare diffusion coefficient.

B. Corrections to the diffusion coefficient

Consider random variations of the channel thickness, which are of Gaussian nature with zero average $\langle h(\mathbf{r})\rangle = 0$ and the correlation function

$$\langle h(\boldsymbol{r})h(\boldsymbol{r}')\rangle_{\mathbf{k}} = \Gamma(|\boldsymbol{k}|), \tag{27}$$

where $\mathbf{k}$ is a wave vector in the longitudinal subspace. We look for the averaged Green's function

$$G(\boldsymbol{r}-\boldsymbol{r}') = \langle G(\boldsymbol{r},\boldsymbol{r}')\rangle = [\hat{G}^0 - \hat{\Sigma}]^{-1}(\boldsymbol{r}-\boldsymbol{r}'), \tag{28}$$

where $G^0(\mathbf{q}) = [-i\omega + Dq^2]$ is the unperturbed solution to Eq. (23) (for $h=0$), and the self-energy part Σ is caused by the perturbation (i.e. h-dependent terms). In the second order in the small variation h, $\Sigma = \Sigma_v + \Sigma_D$ is given by the sum of contributions from the drift term and from the h-dependent part on the rhs of Eq. (25), respectively. These contributions have the form

$$\Sigma_v(\boldsymbol{q}) = \frac{D^2}{V}\sum_{\mathbf{k}} k_\alpha k_\beta \Gamma(k)(k_\alpha - q_\alpha)q_\beta G^0(\boldsymbol{k}-\boldsymbol{q}) \tag{29}$$

and

$$\Sigma_D(\boldsymbol{q}) = \frac{D^2 L_z q_\alpha q_\beta}{V}\sum_{\mathbf{k}} k_\alpha k_\beta \Gamma(k) F(\boldsymbol{k}-\boldsymbol{q}). \tag{30}$$

In the macroscopic limit $\omega,\ q\to 0$, the self-energy part is quadratic in q: $\Sigma \approx -\delta D q^2$, which leads to the renormalization of the bare diffusion coefficient D: $D \to D_{\text{eff}} = D + \delta D$. From Eqs. (29) and (30) we obtain the following contributions to $\delta D = \delta D_v + \delta D_D$:

$$\frac{\delta D_v}{D} = -\frac{1}{dV}\sum_{\mathbf{k}}\Gamma(k) = -\frac{1}{d}\Gamma(\boldsymbol{r}=0) \tag{31}$$

and

$$\frac{\delta D_D}{D} = -\frac{DL_z}{dV}\sum_{\mathbf{k}} k^2 F(k)\Gamma(k). \tag{32}$$

The validity of Eqs. (31) and (32) is restricted to the perturbative case of relatively small corrections. The relative importance of two contributions Eqs. (31) and (32) depends on the ratio between the average channel thickness L_z and the correlation length a of the boundary variations.

1. $a \ll L_z$

In this case of short-range variations the summation over n in Eq. (26) may be substituted by an integration, so that $F(k) \approx F(0) = 1/(Dk)$ and we obtain,

$$\delta D_D/D = -L_z/(dV)\sum_{\mathbf{k}} k\Gamma(k). \tag{33}$$

This contribution is by a factor $L_z/a \gg 1$ greater than Eq. (31). This means that for short-range boundary variations the "fluctuations of the diffusion coefficient" [h-dependent terms in (25)] in Eq. (23) prevail.

2. $a \gg L_z$

The summation over $\mathbf{k}$ in Eq. (32) is restricted to $\mathbf{k} < 1/a \ll 1/L_z$, so that $F(k) \approx F(0) = L_z/(3D)$, and we obtain,

$$\frac{\delta D_D}{D} = -\frac{L_z^2}{3dV}\sum_{\mathbf{k}} k^2\Gamma(k). \tag{34}$$

Apparently, this contribution is by a factor $(L_z/a)^2 \ll 1$ smaller than Eq. (31). We have arrived at the conclusion that for relatively smooth variations the drift term in Eq. (23) is the leading one, while the h-dependent terms in Eq. (25) are irrelevant. This statement remains valid also for nonsmall but smooth boundary variations that are considered in the following section. Note that Eq. (31) together with the expansion $\Sigma \sim q^2$ is valid under the assumption that sums over wave vectors $\boldsymbol{k}$ are well convergent at small $\boldsymbol{k}$ (convergence at large $\boldsymbol{k}$ is always implied). This means that the boundary variations are not too long-range correlated in space. The case of anomalously long-range correlations [e.g., $\Gamma(k) \sim 1/k^2$ in the two-dimensional $(d=2)$ case, which corresponds to the model 3 of [2,4]] needs more care. The contribution of the drift term not only is the dominant one, but it is so large that the perturbation treatment should be substituted by a more sophisticated renormalization group (RG) analysis. Due to the established mapping of the original problem of the variable thickness channel on the problem of the diffusion in an unbounded space with frozen random drifts, the corresponding RG analysis [2–4] developed for the latter problem is directly applicable to the former problem.

IV. SMOOTH BOUNDARY VARIATIONS

In contrast with previous section, here we do not assume smallness of boundary variations. Instead, we assume the function $f(\boldsymbol{r})$ to be smooth on the scale $L_z \sim f$: $\partial_\alpha f \ll 1$. This allows for the adiabatic approximation in Eq. (19),

$$\mathcal{G}_n(\boldsymbol{\rho},\boldsymbol{\rho}') = \frac{(-1)^n L_z}{\pi^2 n^2} \hat{V}_{L_z}(\boldsymbol{\rho}) \mathcal{G}(\boldsymbol{\rho},\boldsymbol{\rho}'). \tag{35}$$

Using Eqs. (35), (18), and (22), we arrive at an effective diffusion equation in d-dimensional subspace. This equation has the standard form (23), with the drift velocity and the diffusion coefficient determined by

$$v_\alpha(\boldsymbol{r}) = D \partial_\alpha \ln f(\boldsymbol{r}) \tag{36}$$

and

$$\hat{D}_{\alpha,\beta}(\boldsymbol{r}) = D[\delta_{\alpha,\beta} - \partial_\alpha f(\boldsymbol{r}) \partial_\beta f(\boldsymbol{r})/3]. \tag{37}$$

In case of small and smooth boundary variations, these expressions coincide with Eqs. (24) and (25), respectively. As has been shown in the previous section, in case of smooth variations the space-dependent fluctuations of the diffusion coefficient are irrelevant, and the macroscopic kinetic coefficients are mainly influenced by the drift term.

It may be shown that Eq. (36) remains valid also for the case of smooth variations of both upper and lower channel boundaries with the function $f(\boldsymbol{r})$ equal to the variable channel thickness. In general, channels bounded in several dimensions with smoothly varying boundaries are described by the same effective diffusion equation (23) with the drift term (36), where $f(\boldsymbol{r})$ is the varying cross section of the channel. Below we shall consider an important particular case of a one-dimensional channel ($d=1$) that allows for a more detailed analytical treatment.

V. ONE-DIMENSIONAL CHANNEL WITH SMOOTHLY VARYING CROSS SECTION

A. Current through the channel

Consider a one-dimensional channel of length L with smoothly varying cross section $f(x)$ (x—the coordinate along the channel, $0<x<L$). For this particularly simple case we shall rederive the basic equations by means of a simple physical reasoning. Namely, we take into account that for a long channel ($L \gg L_z$) the density ρ of diffusing particles is almost constant in the transverse direction and is a smoothly varying function $\rho(x)$ of the longitudinal coordinate. The current density in x direction is given by

$$j_x(x) = \mu F \rho(x) - D \partial_x \rho(x), \tag{38}$$

where we introduced also a constant force F acting on the particles; μ is the mobility connected with D by the Einstein relation $\mu=\beta D$, $\beta=1/k_B T$. The total current through the channel is given by

$$I(x) = f(x)[\mu F \rho(x) - D \partial_x \rho(x)]. \tag{39}$$

Introducing an effective one-dimensional particle density $n(x)=f(x)\rho(x)$, we may rewrite Eq. (39) in the following form:

$$I(x) = [\mu F + D \partial_x \ln f(x)] n(x) - D \partial_x n(x). \tag{40}$$

For $F=0$, the drift term in the above expression corresponds to Eq. (36). For simplicity, in the derivation of the effective diffusion equation (23) with the drift and diffusion terms given by Eqs. (36) and (37), we did not consider an external force. The generalization for a nonzero external force is straightforward and the strict derivation leads to a modification of the drift term (36) $v_\alpha \to v_\alpha + \mu F_\alpha$ in exact correspondence with the heuristically derived Eq. (40).

Below we shall consider the stationary diffusion regime, where the current $I(x)=I$ is constant. In the drift term (40) of the effective equation for diffusion through the channel, the cross-section variations of the original boundary problem enter as an intrinsic force field that corresponds to an effective potential energy $U(x) = -k_B T \ln f(x)$. As is known [12,13], the stationary one-dimensional diffusion problem in an arbitrary potential field allows for an exact solution. We shall derive explicit expressions for the current flowing through the channel under the applied force. We shall also demonstrate a difference between responses of open and closed channels.

B. Open channel

Consider a channel that connects two reservoirs with a given particle density ρ_0. Integrating Eq. (39), we obtain the following general solution:

$$\rho(x) = \rho(0)\exp(-\beta F x) - \frac{I}{D}\int_0^x \frac{dx'}{f(x')} \exp[-\beta F(x-x')]. \tag{41}$$

Using the condition $\rho(0)=\rho(L)=\rho_0$, we arrive at the expression for the current flowing through the open channel,

$$I = D\rho_0 \frac{1-\exp(-\beta F L)}{\displaystyle\int_0^L \frac{dx}{f(x)} \exp[-\beta F x]}. \tag{42}$$

In case of a small external field, when $FL \ll k_B T$, Eq. (42) is approximated by the linear response expression:

$$I^{(1)} = \frac{D\rho_0 F}{\displaystyle\int_0^L \frac{dx}{f(x)}}. \tag{43}$$

Note the following remarkable fact: within the framework of the standard linear diffusion equation, where the bare mobility and diffusion coefficient are independent of the external force, the nonlinearity of the response current (42) is caused only by variations of the channel cross section $f(x)$. For a channel with a constant cross section, $f(x)=f$, the response (42) coincides with the linear expression (43) *for an arbitrary force F*.

The physical mechanism of the nonlinearity is a change of the particle density inside the channel under the action of an external force. For further references we introduce an ''averaged'' particle density $\overline{\rho}$

$$\overline{\rho}\int_0^L dx f(x)=N=\int_0^L dx\rho(x)f(x), \tag{44}$$

where N is the number of particles inside the channel. Using Eqs. (41) and (42), we obtain

$$\overline{\rho}=\frac{N}{\int_0^L dx f(x)}, \tag{45}$$

$$N=\rho_0\int_0^L dx f(x)\exp(\beta Fx)\left[1-\frac{1-\exp(-\beta FL)}{\int_0^L \frac{dx'}{f(x')}\exp(-\beta Fx')}\times\int_0^L dx f(x)\exp(\beta Fx)\int_0^x\frac{dx'}{f(x')}\exp(-\beta Fx')\right]. \tag{46}$$

In the equilibrium (in the absence of the external force F), the averaged particle density (45) coincides with the particle density in the reservoirs, $\overline{\rho}=\rho_0$ for any channel cross section $f(x)$. For a channel with a constant cross section $f(x)=f$, the equality $\overline{\rho}=\rho_0$ holds also for a nonzero F. However, the equality breaks down for channels of variable cross section, where the averaged density $\overline{\rho}$ (45) depends on F.

C. Closed channel

In contrast to the previous case of an open channel, the number of particles in a closed channel does not depend on the applied field. The field applied along the channel influences only the spatial distribution of particles. The latter is given by the Eq. (41) with the periodic boundary condition $\rho(0)=\rho(L)$ [instead of two conditions $\rho(0)=\rho(L)=\rho_0$ at the edges of an open channel]. Another condition is given by Eq. (44), where $\overline{\rho}$ should be considered as a given quantity (we shall mark it with subindex ''c'' to remind of the closed channel). With the use of these conditions we obtain the following expression for the current flowing along the closed channel:

$$I=D\overline{\rho_c}\frac{1-\exp(-\beta FL)}{\int_0^L\frac{dx}{f(x)}\exp(-\beta Fx)}\int_0^L dx f(x)\times\left[\int_0^L dx f(x)\exp(\beta Fx)-\frac{1-\exp(-\beta FL)}{\int_0^L\frac{dx}{f(x)}\exp(-\beta Fx)}\times\int_0^L dx f(x)\exp(\beta Fx)\int_0^x\frac{dx'}{f(x')}\exp(-\beta Fx')\right]^{-1}. \tag{47}$$

In the limit of a weak external field ($FL\ll k_BT$), the linear response of the closed channel coincides with the corresponding expression (43) for the open channel, where ρ_0 should be replaced by $\overline{\rho_c}$.

Similarly, for the case of a channel with constant cross section $[f(x)=f]$, the response (47) to an arbitrary field F coincides with the corresponding linear response expression, quite analogously to the previously considered situation of an open channel. This has a natural explanation: a uniform field F applied to a channel of constant cross section does not change the uniform particle distribution so that the induced current is linear in F.

However, in general, the functional dependences of the induced current (47) on F in open, Eq. (42), and closed, Eq. (47), channels are basically different. This difference exhibits in the nonlinear regime.

Note that using Eq. (45) for the averaged density inside an open channel, the expression (42) for the induced current may be represented in the form (47). This means that being written in terms of actual averaged densities ($\overline{\rho}$ and $\overline{\rho_c}$, respectively), the expressions for induced currents in an open and a closed channels coincide. But the coincidence is only formal, because the quantities $\overline{\rho}$ and $\overline{\rho_c}$ have quite different behavior: the former one does and the latter one does not depend on the external field F. For instance, if the closed channel has been originally in equilibrium with a reservoir of particles with density ρ_0 and has been isolated from the reservoir before applying the external force, the averaged density inside the closed channel would be $\overline{\rho_c}=\rho_0$, and obviously, expressions (42) and (47) for the induced currents would be completely different.

VI. DISCUSSION AND CONCLUSION

We have studied ''confinement'' effects in diffusion of classical particles in channels with varying boundaries. The problem is characterized by the Neumann boundary condition (zero normal flux) in contrast to the Dirichlet boundary condition (zero function) for the quantum confinement problem. Eliminating transverse modes, we have derived an effective diffusion equation (23) that describes particle propagation in an unbounded space of reduced dimension. The equation contains a spatially modulated diffusion coefficient and a frozen field [Eq. (24) or (36)] of drift ''forces'' (velocities), which stem from boundary variations of the original boundary problem. Thus, the original boundary problem, Eqs. (1) and (2), is mapped on a simpler and more customary problem Eq. (23) of classical diffusion in an unbounded medium in the presence of a frozen velocity field. The arising velocity field [Eq. (24) or (36)] corresponds to potential flows, which is the consequence of the Hermitian nature of the original boundary problem. This reduction of the complicated original boundary problem (1) and (2) may be performed for small or smooth boundary variations.

We have shown that random variations of the channel boundary result in a renormalization of an effective diffusion coefficient for disorder averaged propagation. In particular, long-range correlated variations of the channel boundary may result in a subdiffusion regime in accordance with earlier findings for the unbounded diffusion in the presence of random potential flows [2–4].

Furthermore, we have considered in more detail the particular case of stationary diffusion through an effectively one-dimensional channel under the action of an external force. Spatial variations of the channel cross-section result in a nonlinearity of the response current (42) and (47) even for field independent bare values of kinetic parameters (the diffusion coefficient and mobility). This effect is absent for channels with a constant cross section where the current depends linearly on the applied field. The nonlinearity is caused by the field induced redistribution of particles over the channel of varying cross section.

We have shown also that there is a remarkable difference in nonlinear responses of open, Eq. (42), and closed, Eq. (47), channels to an external force. This effect (vanishing in the linear regime) may be considered as a classical analog of a persistent difference in some physical properties of open and closed mesoscopic samples [8,9]. The obtained results are important for the correct interpretation of experiments on particle diffusion through channels of varying cross section.

The mobility and diffusion coefficient renormalization, caused by the channel boundary variations, may be considered as a classical analog to quantum weak localization effects in channels with spatially varying confinement energy. The classical problem may arise also as a part of the quantum diffusion problem in disordered channels (waveguides) with a smoothly varying boundary: the first averaging over the disorder leads to a finite mean free path l and the particle motion is described by diffusion propagators. These propagators, in turn, should be averaged over ''macroscopic'' variations of the channel geometry. A related problem, that may also be considered as the classical analog of a corresponding ''quantum'' one, is the problem of the energy level statistics of the classical diffusion operator in closed samples with corrugated boundaries and the Neumann boundary condition. As noted above, this problem may arise as a classical part of the quantum problem on the level statistics of the Schrödinger equation in disordered samples with boundaries smoothly corrugated on the scale of the mean free path [14].

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