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Ballistic Transport in Narrow Channels and Films

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We present a simple description of ballistic transport in systems with random rough walls. All characteristic parameters, including the mean free path and localization length, are expressed explicitly via the correlation function (correlation length R and amplitude ℓ) of surface inhomogeneities. Scattering by surfaces inhomogeneities in channels with width L creates a new mesoscopic transport length of the order of $\left(L^2 R/\ell^2\right) f\left(R/\lambda\right)$. The function f has a minimum when the particle wavelength $\lambda \sim R$. The transport problem includes possible quantization of motion across the channel. The calculations are performed with the help of canonical coordinate transformation which reduces a transport problem with rough random walls to an exactly equivalent problem with ideal flat walls, but with random bulk distortion. Applications include transport in thin films, porous media, localization and slip effects, etc.

1. INTRODUCTION

Boundary scattering is important for many branches of physics especially at low temperatures when the (quasi-)particle mean free paths are large. Boundary roughness leads to chaotization of motion and additional diffusion along the walls. This transport effect should be described in terms of correlation function of surface inhomogeneities. However, such a description is still missing, at least in an accurate and consistent form. Below we solve this long-standing problem for ballistic particles.

Usually, boundary problems are studied using either an "exact" boundary condition which leads to an unsolvable integro-differential transport problem, or an over-simplified Fuchs boundary condition which balances specular and diffuse reflection. One can also[1–3] substitute the boundary roughness by some random bulk potential near the surface, and to express the transport characteristics via the parameters of this potential. Though this approach reproduced many features of transport processes, the effective potential remained unknown and could not be reconstructed neither theoretically nor experimentally.

We developed a different approach. We use a canonical coordinate transformation (similar to the Migdal transformation in nuclear physics) so that to make the boundaries flat, and look for the effect of this transformation on transport. [Similar transformation was used earlier[4–7] for diffraction patterns of electromagnetic and acoustic waves near rough surfaces]. As a result of this transformation, the *bulk* Hamiltonian acquires additional random terms which contain the information on boundary roughness. This *bulk* distortion is expressed via the shape of the surface and has a much more complicated functional and operator structure than the effective potential in Refs.[1–3] The bulk distortion can be introduced into perturbative collision integral, which, in turn, can be translated into transparent expressions for transport coefficients. The formalism is very simple even in rather convoluted situations. We are able to express all transport characteristics explicitly through the shape of the rough surface, *i.e.*, the correlation function of surface inhomogeneities. Some preliminary results were recently published in[8] (see also[9]).

We will neglect all bulk relaxation processes. Then the random boundary scattering becomes the main source of the formation of the mean free path along the walls. The method can be applied to thin films, narrow channels, ballistic transport in porous media with high porosity, localization and mesoscopic effects, *etc.*

2. COORDINATE TRANSFORMATION AND BULK HAMILTONIAN

We consider a film (or a $1D$ channel) of the average thickness L with the boundaries $x = \pm L/2 \mp \xi_{1,2}(y,z)$ with small random inhomogeneities, $\xi_1, \xi_2 \ll L$, $\langle \xi_1 \rangle = \langle \xi_2 \rangle = 0$. Since there is no bulk relaxation, the results depend only on the function $\xi(\mathbf{s}) = \xi_1(\mathbf{s}) + \xi_2(\mathbf{s})$, *i.e.*, on the correlation function $\zeta(\mathbf{q}) = \zeta_{11} + \zeta_{22} + 2\zeta_{12}$,

$$\zeta_{ik}\left(|\mathbf{s}_1 - \mathbf{s}_2|\right) = \langle \xi_i(\mathbf{s}_1)\xi_k(\mathbf{s}_2)\rangle, \ \zeta_{ik}(\mathbf{q}) = \int d^2s\, e^{i\mathbf{q}\cdot\mathbf{s}/\hbar}\zeta_{ik}(\mathbf{s}) \tag{1}$$

We will study Gaussian correlation function,

$$\zeta(s) = \ell^2 \exp\left(-s^2/2R^2\right), \ \ \zeta(\mathbf{q}) = 2\pi\ell^2 R^2 \exp\left(-q^2R^2/2\hbar^2\right) \tag{2}$$

and its δ-type limit for very small correlation radius R, $\zeta(s) = \ell^2 R^2 \delta(s)/s$.

The coordinate transformation

$$X = \frac{L[x - \frac{1}{2}(\xi_2(y,z) - \xi_1(y,z))]}{L - (\xi_1(y,z) + \xi_2(y,z))}, \ Y = y, \ Z = z \tag{3}$$

makes the both boundaries flat, $X = \pm L/2$. This transformation should be supplemented by the conjugate transformation of momenta,

$$p_x = P_x \frac{L}{L - \xi(y,z)},\ p_y = P_y + P_x \frac{X\xi_y' + \frac{1}{2}L(\xi_{2y}' - \xi_{1y}')}{L - \xi_1(y,z)}, \tag{4}$$

and the same for p_z ($\xi_{1,2y} = \partial\xi_{1,2}/\partial y$). In new variables, the quadratic Hamiltonian acquires some random "perturbation" $\widehat{V}$, $\widehat{H} = \widehat{p}^2/2m = \widehat{P}^2/2m + \widehat{V}$ with $\left\langle \widehat{V} \right\rangle = 0$. In relatively thick and smooth films, ξ/L, $\xi_{1,2y}', \xi_{1,2z}' \ll 1$,

$$\widehat{V} = \frac{\xi}{mL}\widehat{P}_x^2 + \frac{1}{2m}\left(X\widehat{P}_x \frac{\xi_y'}{L}\widehat{P}_y + X\widehat{P}_x \frac{\xi_z'}{L}\widehat{P}_z + H.c. \right) \tag{5}$$

Note, that the exact Hamiltonian contains not only the perturbation $\widehat{V}$ (5), but some extra terms with $\xi_1' - \xi_2'$. However, in the absence of bulk relaxation, these terms disappear from the transport equation.

In the ultra-quantum case (thin films), the motion across the film is quantized with $P_x = \pi\hbar j/L$. The distance between states with different j can be so large that the interstate transitions are effectively suppressed. Then the motion of particles along the film is $2D$ motion in states j in some random potentials $V^{(j)}$. When $P_x = \pi\hbar j/L$ is much larger than the momentum along the film $\mathbf{Q} = (P_y, P_z)$

$$V^{(j)}(y,z) \simeq \left(\frac{\pi j\hbar}{L}\right)^2 \frac{\xi(y,z)}{mL} \tag{6}$$

If $P_x = \pi\hbar j/L \gg Q$, but the interstate transitions are not suppressed, one cannot ignore the terms with Q in Eq.(5).

In classical mechanics the Hamiltonian (5) is equivalent to random coordinate-dependent anisotropic effective mass,

$$\left(\frac{1}{m_{eff}}\right)_{xx} = \frac{1}{m}\left(1 + \frac{2\xi}{L}\right),\ \left(\frac{1}{m_{eff}}\right)_{xy} = \frac{X\xi_y'}{mL},\ \left(\frac{1}{m_{eff}}\right)_{xz} = \frac{X\xi_z'}{mL} \tag{7}$$

This analogy can be useful for numerical analysis of transport.

3. TRANSPORT COEFFICIENTS

The perturbative collision integral for particles with Hamiltonian (5)

$$L_{coll} = \int W(\mathbf{P}, \mathbf{P}')\left[n(1-n') - n'(1-n)\right] d^3P'/(2\pi\hbar)^3 \tag{8}$$

is determined by the probability of transitions between states with different momenta (averaged over ξ) $W(\mathbf{P},\mathbf{P}')$, which, in turn, is given by the square of the matrix element of the perturbation (5). For (quasi-)classical motion,

$$W(\mathbf{P},\mathbf{P}') = \frac{\zeta(\mathbf{Q}-\mathbf{Q}')}{4\pi L^2 m^2}\delta(\epsilon-\epsilon')\times \left[2P_x^4\delta(P_x-P_x') + \Omega P_x^2\delta'(P_x-P_x') + \frac{\Omega^2}{8}\delta''(P_x-P_x')\right]$$

In the ultra-quantum case with discrete states j for the motion across the channel and suppressed interstate transitions, the collision integrals L_j are

$$L_j = \frac{1}{2\pi\hbar^3 m^2 L^2}\int d^2Q'\,\zeta(\mathbf{Q}-\mathbf{Q}')\sum_{j'}\left(n_{j'}(\mathbf{Q}') - n_j(\mathbf{Q})\right)\delta\left(\epsilon_{j'\mathbf{Q}'}-\epsilon_{j\mathbf{Q}}\right) \times\left[\delta_{jj'}\left(\frac{1}{4}(\mathbf{Q}-\mathbf{Q}')^2 + \left(\frac{\pi\hbar j}{L}\right)^2\right)^2 + \frac{(1-\delta_{jj'})\,j^2 j'^2}{(j^2-j'^2)^2}\left(Q'^2-Q^2\right)^2\right]$$

In the classical case the conductivity of Boltzmann particles is

$$\sigma = \frac{32}{\pi^{3/2}}\frac{e^2L^2R^2N}{\hbar\ell^2}xf_B(x),\ x = \frac{\hbar}{(4mT)^{1/2}R}, \tag{9}$$

while in degenerate systems

$$\sigma = \frac{\sqrt{2}e^2L^2}{\pi^3\hbar\ell^2R}x^2f_F(x),\ x = \sqrt{2}\frac{p_FR}{\hbar} \tag{10}$$

Functions $f_B(x)$ and $f_F(x)$ (Figs.1,2) are some hypergeometric integrals. Both functions $f_{B,F}(x)\to\infty$ for $x\to 0$ and $x\to\infty$. Eqs.(10) correspond to the following effective surface-induced mean free paths $\mathcal{L}$ along the film:

$$\mathcal{L}_B = \frac{16}{\pi^{3/2}}\frac{L^2R}{\ell^2}f_B(x),\ \mathcal{L}_F = \frac{12\sqrt{2}}{\pi}\frac{L^2R}{\ell^2}f_F(x) \tag{11}$$

The argument of the functions $f_{B,F}(x)$ is the ratio of the de Broglie wavelength λ to the correlation radius of the surface inhomogeneities R, and the wall-induced mean free path is $\mathcal{L}\sim\left(L^2R/\ell^2\right)f(R/\lambda)$. The mean free path and the transport coefficients are quadratic in the film thickness; this conclusion agrees with experimental data.[1,10]

It is not surprising that the most effective chaotization of motion (the shortest mean free path) occurs at $R/\lambda\sim 1$. The long-wave limit $R/\lambda\to 0$ corresponds to quantum reflection of particles when functions $f_{B,F}$ increase and $\mathcal{L}\to\infty$. This is a transport manifestation of the fact that reflection of

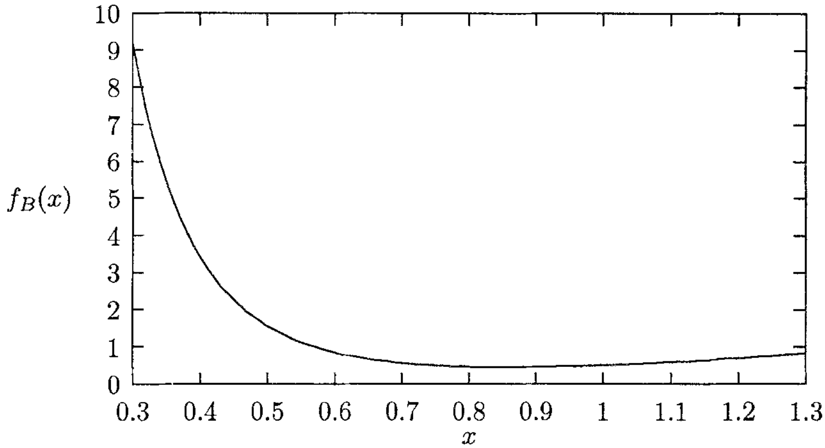

Fig. 1. Function $f_B(x)$

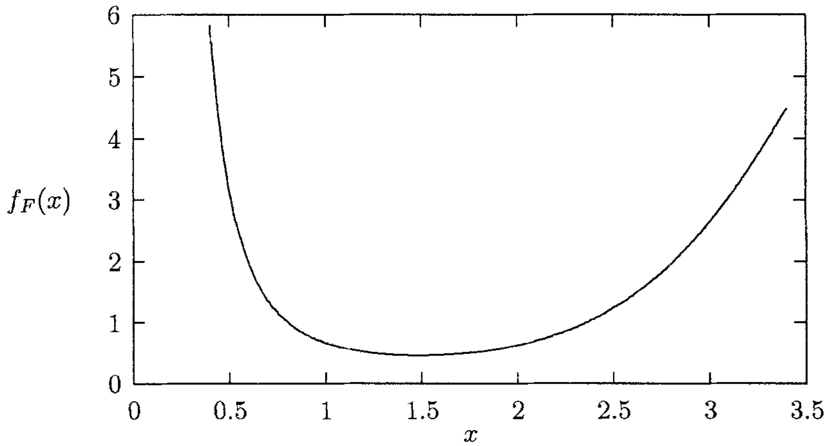

Fig. 2. Function $f_F(x)$

long-wave particles is effectively specular. In the opposite case, $R/\lambda \to \infty$, the increase of the mean free path means that the reflection from wider (smoother) inhomogeneities is also specular.

In the ultra-quantum case of very thin films, the conductivity of degenerate particles on each quantum level is

$$\sigma_{xx}^{(j)} = \sigma_{yy}^{(j)} = \frac{e^2 L^2 \hbar^3 N^{(j)}}{16\pi \ell^2 R^2} \left(\frac{L}{\pi \hbar j}\right)^4 \frac{1}{{}_1F_1\left(\frac{3}{2}, 2, -4\pi N^{(j)} R^2\right)},$$

(for Boltzmann distribution the expression is similar).

Other transport coefficients are calculated in the same way. In essence, we calculated the mean free path $\mathcal{L}$ along the surface imposed by scattering of particles by surface inhomogeneities. This information on wall-induced mean free path and diffusion coefficients is sufficient for description of localization processes and quantum interference corrections to transport. For example, the localization length for different quantum states in thin films is $\mathcal{R}^{(j)} \sim \mathcal{L}^{(j)} \exp\left(\pi^2 \mathcal{L}^{(j)}/\lambda\right)$. On the other hand, the scattering by random boundary inhomogeneities can play the role of elastic "impurity" scattering necessary for the formation of unusual localization regime[11] in quantum dots with different length scales in different directions.

More detailed results will be published in.[9] The work was supported by NSF grant DMR-9412769.

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