Transport in Channels and Films with Rough Surfaces. II. Quantized Motion of Ballistic Particles

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(October 18, 1995)

This is the second in the series of papers on transport phenomena along random rough surfaces.

We apply our simple general approach [1] to transport in very narrow channels, when the particles wavelength is comparable to the width of the channels and the motion across the channel is characterized by discrete quantum states. The discrete nature of the spectrum leads to a non-analyticity of transport coefficients as a function of thickness or channel width, especially for degenerate fermions. Surface inhomogeneity leads to both on-level scattering and interlevel transitions. As in [1], transport coefficients are expressed explicitly via the correlation function of surface inhomogeneities. The shape of the curves for the dependence of transport coefficients on the number of particles and/or film thickness is determined by the correlation radius of surface inhomogeneities and is not sensitive to their amplitude. For short range correlations, the curves assume a saw-like shape as a result of the interlevel transitions. With increasing correlation radius, the interlevel transitions lose their importance, and the saw teeth gradually decrease, reducing, in the end, to simple kinks on practically monotonic curves. Applications include Gaussian and short-range $\delta$-type correlations. Careful analysis of the transition from quantum to semi-classical and classical regimes allowed us to improve the accuracy of our previous classical calculations.

PACS numbers: 72.10.Bg, 73.20.Fz, 73.50.Bk, 79.20.Rf

I. INTRODUCTION

Repeated collisions of (ballistic) particles with rough walls with random inhomogeneities result in gradual chao-

tization of motion of particles along the walls, and lead to formation of the mean free path. Though this is a very old problem, important for different branches of physics, a simple consistent description has been absent. Recently we suggested a new simple quantitative approach to transport phenomena in systems with rough walls [1] (referred below as I; see also [2]). Within this approach, one can easily express transport and localization parameters (such as mobility, diffusion, mean free path, localization length, etc.) for the motion of ballistic particles along the walls directly via the correlation function of wall inhomogeneities. The only restriction is that the inhomogeneities should be relatively smooth with the amplitude $\ell$ smaller than their correlation radius $R$ and the thickness of the film (width of the channel) $L, \ell \ll L, R$.

Our approach is based on the use of an explicit canonical coordinate transformation (similar to the Migdal transformation in nuclear physics) which makes the initially rough boundaries flat. The price is a considerable complication of the bulk transport equation which, however, can be treated perturbatively. This transformation corresponds to stretching of the film (channel) width with the stretching parameters changing along the film in accordance with the exact shape of the boundaries. Since, in contrast to earlier, more heuristic approaches [3,4], we are using an explicit expression for the coordinate transformation with the parameters given by the exact profile of the random boundaries, our reformulation of the transport problem with random rough walls as the transport problem with flat walls and randomly distorted bulk, is exact. The latter problem allows a straightforward perturbative solution which involves averaging over initial boundary inhomogeneities.

In many cases, all the calculations after the coordinate transformation are really very simple and straightforward. In I we illustrated our method for a wide range of the problems. In this paper we will concentrate on the case of very thin films and narrow channels when the motion of (longwave) particles across the channel is quantized with a noticeable separation between the states.

One of the effects that we want to describe is the following. In thin films with discrete levels for motion across the film, the increase in particle density and/or film thickness cause redistribution of particles between levels. In Fermi systems at $T \to 0$ this is a non-analytical step-like process. In this case, the lower levels are filled, while the higher levels are unoccupied. The (gradual) change in the total number of particles results, at certain critical values, in the change of the number of occupied levels by one. These abrupt changes in the number of occupied levels should lead to a non-analytical dependence of the density of states and other thermodynamic functions on the number of particles. Obviously, this effect should also lead to singularities in the dependence of the transport coefficients on film thickness or density of particles. This saw-like effect has already been described in the case of bulk scattering [1], and has
been qualitatively suggested in Ref. [4] for scattering by rough walls. We will be able to get quantitative results, and express explicitly the transport singularities via the correlation function of surface inhomogeneities.

What is more, we will demonstrate that the picture is even more interesting than in Ref. [4]. We will see that the particle transport along the film is a non-trivial function of two parameters, \(NL^2\) and \(L/R\), where \(L\) is the thickness of the film with the 2D density of particles \(N\), and \(R\) is the correlation radius of surface inhomogeneities. The saw-like dependence of the transport coefficients on \(NL^2\) is well-pronounced only for short-range correlations of surface inhomogeneities, \(NR^2 \ll 1\). With an increase of the correlation radius \(R\), the saw-like structure of the curves will gradually disappear, and the curves will become more and more smooth. It turns out that the saw-like shape of the curves is associated exclusively with the interlevel transitions the rate of which is determined by the parameter \(NR^2\); if one artificially forbids the interlevel transitions even at small \(NR^2\), the curves will lose their saw-like character and will become similar to those at large \(NR^2\).

Of course, the density dependence of transport coefficients becomes more and more smooth with increasing temperature even though the energy spectrum remains distinctly discrete.

In the next Section we will present general equations for quantized transport in thin films with rough boundaries. Then, in Sec.3, we will study transport singularities for degenerate fermions at \(T = 0\). In Sec.4 we will derive the corresponding transport equations for finite temperatures, and calculate the transport coefficients in Boltzmann temperature range. Our detailed analysis of transport of particles with discrete spectrum will demonstrate that the accuracy of previous calculations for continuous spectrum (\(i.e., \) in classical and/or semi-classical limit) in I can be improved considerably. The consistent transition from discrete to continuous expressions will provide us with much more accurate expressions for the squares of the \(\delta\)-functions, which appear in the calculations of the squares of the matrix elements, than the approximations used in purely classical calculations I. The improved classical transport calculations will be described in the Appendix.

II. QUANTIZED STATES ACROSS THE CHANNELS

As in I, we will consider a film (channel) of the average thickness \(L\) with rough boundaries \(x = L/2 - \xi_1(y, z)\) and \(x = -L/2 + \xi_2(y, z)\). The small boundary inhomogeneities, \(\xi_1, \xi_2 \ll L\), are random functions of coordinates \(s = (y, z)\) along the boundaries, \(\langle \xi_1 \rangle = \langle \xi_2 \rangle = 0\), with the correlation function

\[
\zeta_{ik}(|s_1 - s_2|) = \langle \xi_i(s_1)\xi_k(s_2) \rangle , \tag{1}
\]

\[
\zeta_{ik}(q) = \int d^2s \ e^{iqs/h} \zeta_{ik}(s)
\]

where \(q\) is the momentum along the wall. In homogeneous systems, the correlation function depends only on the distance between points \(|s_1 - s_2|\) and not on coordinates themselves. In the absence of the bulk relaxation, the results, as in I, depend only on the function \(\xi(s) = \xi_1(s) + \xi_2(s)\) and the correlation function \(\zeta(|s_1 - s_2|) = \langle \xi(s_1)\xi(s_2) \rangle = \xi_{11} + \xi_{22} + 2\xi_{12} \).

Though we can calculate the transport coefficient for arbitrary correlation function \(\zeta(s)\), we will supplement general expressions by the most practical examples of Gaussian correlations of the surface inhomogeneities of an average height \(\ell\),

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

including the limiting case of the very small correlation radius \(R\), \(i.e.,\) the \(\delta\)-type correlations,

\[
\zeta(s) = \ell^2R^2\delta(s)/s , \quad \zeta(q) = 2\pi\ell^2R^2 \tag{3}
\]

Note, that the condition \(\ell \ll R\) does not mean that our approach is applicable to long-range correlations (large size inhomogeneities) exclusively. The scale for the effective correlation range in Eq.(2) is defined by the particles wavelength \(\lambda\). For longwave particles \(\lambda \gg R\) one deals effectively with the short-range \(\delta\)-type correlations (3), while in the opposite case of long-range correlations \(\lambda \ll R\) one should consider the full Gaussian expression (2).

Our approach is based on the use of canonical coordinate transformation

\[
X = \left. \frac{L|x - \frac{1}{2}(\xi_2(y, z) - \xi_1(y, z))|}{L - (\xi_1(y, z) + \xi_2(y, z))} \right|, \quad Y = y, \quad Z = z \tag{4}
\]

which corresponds to the following change of the form of the bulk Hamiltonian \(\tilde{H} = \frac{p^2}{2m}\):
\( \hat{H} = \frac{\hat{p}_x^2}{2m} + \hat{V}, \quad \hat{V} = \frac{\xi}{mL} \hat{p}_x^2 + \frac{1}{2m} \left( X \hat{p}_x \frac{\xi_y}{L} \hat{p}_y + X \hat{p}_y \frac{\xi_y}{L} \hat{p}_x + H.c. \right) \) \tag{5}

(for details see I). The randomness of inhomogeneities, \( \langle \xi \rangle = 0 \), leads to the randomness of the bulk "perturbation" \( \hat{V} \), \( \langle \hat{V} \rangle = 0 \). Thus, the transformation \( \hat{\Phi} \) reduces the transport problem between rough walls to an equivalent transport problem with ideal specular walls, \( \Psi(L/2) = \Psi(-L/2) = 0 \), but with a distorted bulk Hamiltonian \( \hat{\Phi} \). The latter problem can be treated in the same standard perturbative way as for any random bulk imperfections or impurities.

In thin films, the motion of particles across the films is quantized, \( \xi \hat{q} \hat{\xi} \). Then the wave functions which correspond to the unperturbed problem can be treated in the same standard perturbative way as for any random bulk imperfections or impurities. The transition between them are practically forbidden. Then the transport problem reduces to independent calculations of the mean free paths \( \ell \) for each level. The randomness of inhomogeneities, \( W \), the transition probabilities are given by the squares of the matrix elements of the perturbation \( \hat{\Phi} \):

\[ \int W_{jj'}(\xi, \xi') \left[ n_j(1-n_{j'}) - n_{j'}(1-n_j) \right] \frac{d^2 q'}{(2\pi \hbar)^2} \]

The transition probabilities are given by the squares of the matrix elements of the perturbation \( \hat{\Phi} \):

\[ W_{jj'}(\xi, \xi') = \frac{2\pi}{\hbar} \left| \langle \xi | \hat{\Phi} | \xi' \rangle \right|^2 \delta (\epsilon_j(\xi) - \epsilon_{j'}(\xi')) \] \tag{9}

Since all the equations include only the squares of the matrix elements of the "perturbation" \( \hat{\Phi} \), the averaging over the random surface inhomogeneities does not cause any problems leading directly to the correlation function \( \zeta(s) \).

The matrix elements of the perturbation \( \hat{\Phi} \) are

\[ V_{\xi, \xi'} = V_{\xi, \xi'}^{(x)} + V_{\xi, \xi'}^{(y)} + V_{\xi, \xi'}^{(z)} \]

\[ V_{\xi, \xi'}^{(x)} = \frac{\delta_{jj'}}{2m L \xi} (j^2 + j'^2) \xi(\xi - \xi') \]

\[ V_{\xi, \xi'}^{(y)} = \frac{(-1)^{j+j'}(j^2 + j'^2)}{2m L \xi} \xi(\xi - \xi') (q_y' - q_y) \times \left[ q_y' \left( \frac{1}{j+j'} + \frac{1}{j-j'} (1 - \delta_{jj'}) \right) - q_y \left( \frac{1}{j+j'} - \frac{1}{j-j'} (1 - \delta_{jj'}) \right) \right] \]

and the collision integral for particles on each level \( j \) becomes, after averaging over inhomogeneities, equal to

\[ L_j = \frac{1}{2\pi \hbar^3 m^2 L^2} \int d^2 q' \zeta(\xi - \xi') \sum_{j'} (n_{j'}(\xi') - n_j(\xi)) \delta (\epsilon_{j'}(\xi') - \epsilon_{j}(\xi)) \times \left[ \delta_{jj'} \left( \frac{1}{4}(\xi - \xi')^2 + \left( \frac{\pi \hbar j}{L} \right)^2 \right)^2 + \frac{1}{(j^2 - j'^2)^2} \left( q^2 - q'^2 \right)^2 \right] \] \tag{11
This collision integral includes both on-level scattering (diagonal terms with $\delta_{jj'}$) and interlevel transitions (off-diagonal terms with $1 - \delta_{jj'}$) which are induced by surface roughness.

In I we assumed that the interlevel transitions disappear (i.e., that the off-diagonal terms in (11) can be neglected) with an increase in the distance between levels. We solved the transport equation without interlevel transition with an additional assumption that the film is very thin and, therefore, the components of particle momenta across the film are larger than those along the film, $(\pi \hbar j/L)^2 \gg (\mathbf{q} - \mathbf{q}')^2$. The results below show that these assumptions are self-consistent for large correlation radii of surface inhomogeneities, $NR^2 \gg 1$. For smaller correlation radii the interlevel transitions and momenta along the film cannot be neglected even in the case of large interlevel spacing. As we will see, the approximation I, though valid in important limiting cases, misses the most interesting features of transport through very narrow channels or thin films.

III. SINGULARITIES IN TRANSPORT OF PARTICLES WITH DISCRETE QUANTUM STATES: LOW TEMPERATURES

Changes in particle density and/or thickness of the film lead to redistribution of particles between discrete quantum states $j$. This redistribution between discrete states may lead to a non-analytic dependence of transport coefficients on particle density and thickness of the film. Of course, this non-analyticity is more pronounced for degenerate Fermi systems at $T \to 0$ when continuous increase in the number of particles leads, at certain critical densities, to filling of new levels with higher and higher values of $j$. Below we will look at this non-analytic effect in some detail.

At $T = 0$, the Fermi momenta of fermions for the motion along the film $q_F^{(j)}$ on each level $j$ are given by the overall Fermi energy (chemical potential) $\epsilon_F$ as

$$\epsilon_F = \frac{1}{2m} \left( \left( \frac{\pi j \hbar}{L} \right)^2 + q_F^{(j)^2} \right)$$  \hspace{1cm} (12)

while the 2D density of spin-1/2 particles on each level is

$$N_j = \frac{q_F^{(j)^2}}{2\pi \hbar}$$  \hspace{1cm} (13)

(for simplicity we assume that the effective masses of particles on all levels are the same). The chemical potential $\mu = \epsilon_F$ should, as usually, be determined self-consistently by calculating the total density of particles $N$,

$$N = \sum_j N_j = \frac{1}{2\pi \hbar^2} \sum_j \left( 2m\epsilon_F - \left( \frac{\pi j \hbar}{L} \right)^2 \right).$$  \hspace{1cm} (14)

Eqs. (12)-(14) in convenient dimensionless notations,

$$\nu = 2m\epsilon_F \left( \frac{L}{\pi \hbar} \right)^2, \ z_j = \frac{2}{\pi} N_j L^2, \ z \equiv \sum_j z_j = \frac{2}{\pi} NL^2,$$  \hspace{1cm} (15)

can be rewritten as

$$z_j = \nu - j^2, \ z = \sum z_j$$  \hspace{1cm} (16)

The number of occupied levels $S$ for the given value of $z$ (i.e., for the number of particles $NL^2$) is given by the integer part of $\nu^{1/2}(z)$,

$$S(z) = \text{Int} \left[ \sqrt{\nu} \right]$$  \hspace{1cm} (17)

All the levels with the indices $j > S$ are empty, $z_{j > S} = 0$. Summation of Eqs. (16) from 1 to $S$ defines the number of occupied levels $S$ and the dimensionless chemical potential $\nu$ as functions of the number of particles $z$:

$$S = \text{Int} \left[ \sqrt{\nu} \right] = \text{Int} \left[ \sqrt{\frac{z}{S} + \frac{(S+1)(2S+1)}{6}} \right],$$  \hspace{1cm} (18)

$$\nu(z) = \frac{z}{S} + \frac{1}{6} (S+1)(2S+1)$$
and can be conveniently parametrized as

\[ S \]

The singular points correspond to change in values of \( S \), where

\[ \Phi(z) \]

...for computational purposes, it is more convenient to start the calculations by defining the number of occupied levels \( S \), and to determine the interval of the values of \( z \) and \( \nu \), which corresponds to this number of levels, basing on the value of \( S \). The changes in number of occupied levels \( S = 1, 2, 3, 4, 5, 6, \ldots \) occur at \( z = 0, 3, 13, 34, 70, 125, \ldots \) (i.e., in the points \( z = S^3 - S(S + 1)(2S + 1)/6 \)).

At \( T = 0 \), we look for the solution of the transport equation (7) in the form

\[ n_j(q) = n_j^{(0)}(q_{F}^{(j)}) - \frac{F L^3}{\pi^4 L^2} \delta(\epsilon - \epsilon_F) \chi_j(q_{F}^{(j)}) \cos \theta_j, \]

where \( \theta_j \) is the angle between the momentum \( q_j \) and the external force \( \mathbf{F} \). Then, after the integration of the collision integral (11) with the Gaussian correlation of surface inhomogeneities (2), the transport equation reduces to the following set of dimensionless linear equations in \( \chi_j(q_{F}^{(j)}) \):

\[ z_j^{1/2} \frac{L^2}{R^2} = -\frac{1}{2} \chi_j \times \]

\[ \left( 4 j^4 \frac{1}{F_1} \left( \frac{3}{2}, 2, -\frac{2\pi^2 z_j R^2}{L^2} \right) + 6 z_j j^2 \frac{1}{F_1} \left( \frac{5}{2}, 3, -\frac{2\pi^2 z_j R^2}{L^2} \right) + 5 \frac{z_j^2}{2} \frac{1}{F_1} \left( \frac{7}{2}, 4, -\frac{2\pi^2 z_j R^2}{L^2} \right) \right) \]

\[ + 2 \sum_{j'} (1 - \delta_{jj'}) j^2 j'^2 \exp \left[ -\pi^2 \left( \sqrt{z_j} - \sqrt{z_{j'}} \right)^2 R^2/2L^2 \right] \times \]

\[ \chi_{j'} \left( \frac{1}{2} \frac{1}{F_1} \left( \frac{1}{2}, 1, -\frac{2\pi^2 \sqrt{z_j z_{j'} R^2}}{L^2} \right) - \frac{1}{2} \frac{1}{F_1} \left( \frac{3}{2}, 2, -\frac{2\pi^2 \sqrt{z_j z_{j'} R^2}}{L^2} \right) \right) - \chi_j \frac{1}{F_1} \left( \frac{1}{2}, 1, -\frac{2\pi^2 \sqrt{z_j z_{j'} R^2}}{L^2} \right) \]

(we will not give here similar cumbersome equations for the correlation function of a general form \( \zeta(q) \)). The conductivity (mobility) of particles is given by the solution of this set of equations,

\[ \sigma_{yy} = \sigma_{zz} = \sum_{j=1}^{S} \sigma_{yy}^{(j)} = \frac{e^2 L^2}{2\pi^4 R^2} \sum_{j=1}^{S} \frac{z_j^{1/2} \chi_j(q_{F}^{(j)})}{\sqrt{z_j}}, \]

and can be conveniently parametrized as

\[ \sigma_{yy}^{(j)} = \sigma_{zz}^{(j)} = \frac{e^2 L^2}{2\pi^4 R^2} \Phi \left( \sqrt{z_j} \frac{L}{R} \right) \]

The functions \( \Phi(z) \) for four different values of \( R/L \) are plotted in Fig. 1 (\( R/L = 0.05 \)) and Fig. 2 (\( R/L = 1; 3; 5 \)). The singular points correspond to change in values of \( S \) from 1 to 2 to 3 to 4... at \( z = 3, 13, 34... \).

![FIG. 1. Function \( \Phi(x) \), Eq. (21), for \( R/L = 0.05 \) (solid line); dashed line - the same function calculated without interlevel transitions](image-url)
Another way of parameterization of equations, similar to the one used in I, is based on definition

$$\frac{2\pi^2 \sqrt{z_j z'_j \lambda^2}}{E^2} = \frac{4\pi \sqrt{z_j z'_j N \lambda^2}}{z} = \frac{8\pi^2 \sqrt{z_j z'_j \lambda^2}}{z} \left(\frac{R}{\lambda}\right)^2,$$

where the effective particle wavelength $\lambda^2 = 2\pi/N$. This equation redefines the function $\Phi(z, L/R)$ as $\tilde{\Phi}(z, \lambda/R) = \Phi(z, \sqrt{2\pi}/2R)$.

Dramatic difference in shapes of the curves in Figs. 1 and 2 for small and large values of $R/L$ is explained by the role of interlevel transitions. If one simply neglects the interlevel transitions (the off-diagonal terms) in the collision integral (11), then the set of transport equations (19) will decouple into $S$ independent equations. It is fairly obvious that in this approximation the conductivity (20) is almost always a monotonic function of $z = 2NL^2/\pi$, though the critical values of $z$, which correspond to the change in the number of occupied levels $S$, are still responsible for the singularities (kinks) in the curves. Therefore, the saw-like nature of the curves is caused by the interlevel transitions exclusively.

For comparison, Fig. 1 (dashed line) and Fig. 3 give the function $\Phi(z)$ for on-level scattering exclusively, i.e., when all the interlevel off-diagonal terms in the collision integral (11) are artificially neglected. Obviously, the curves with and without transitions always coincide as far as $z \leq 3$ and there is only one occupied level. The differences show up only at $z > 3$. 
FIG. 3. Function $\Phi(x)$, Eq. (21), for $R/L = 1/5$ calculated without interlevel transitions.

On the other hand, the importance of interlevel transitions is characterized by the parameter $NR^2 \sim zR^2/L^2$. Since $z_j - z_{j'} = j^2 - j'^2$, the exponent

$$\exp\left[-\pi^2 \left(\sqrt{z_j} - \sqrt{z_{j'}}\right)^2/R^2\right] \equiv \exp\left[-\pi \left(\sqrt{N_j}R^2 - \sqrt{N_{j'}}R^2\right)^2\right]$$

always makes interlevel transitions to remote levels $|j - j'| \gg L/R$ negligible. These exponents show that the interlevel transitions and the resulting mixing of adjacent levels are very important only for not very populated levels with $2\pi^2 z_j R^2/L^2 \ll 1$. Thus, the contribution of interlevel transitions is very noticeable only for relatively small values of $R/L$, and decreases exponentially with increasing $R/L$. For this reason, the saw-like character of particles mobility becomes less and less pronounced with increasing $R/L$. At $R/L = 5$ the saw nearly completely disappears, and there is practically no difference between the curves in Figs. 2 (exact calculation) and Fig. 3 (calculation with artificially neglected interlevel transitions). Note, that the curves calculated with and without transitions always coincide for a small number of particles $z < 3$ when only one level is occupied and the transitions are impossible for energy reasons.

The same parameters, $2\pi^2 z_j R^2/L^2 = 4\pi N_j R^2$, determine the values of the hypergeometric functions in Eq. (19). At $x^2 \ll 1$, $\,_1F_1 \left((2n-1)/2, n, -x^2\right) \simeq 1$, while in the opposite case $x^2 \gg 1$, $\,_1F_1 \left((2n-1)/2, n, -x^2\right) \simeq (n-1)!/\sqrt{\pi x^n}$. Therefore, at large $2\pi^2 z_j R^2/L^2 \gg 1$, one can not only neglect the interlevel transitions, but also the hypergeometric functions with $n = 3$ and $n = 4$ in the diagonal terms of the collision integrals in comparison with the one with $n = 2$. Only under these conditions one can justify a heuristic assumption made in I and recover the result (I.53):

$$\sigma_{yy} = \sum_{j=1}^{S} \sigma_{yy}^{(j)} = \frac{S^2 R^2}{\pi^4 \hbar^2} \Phi \left(\frac{z}{R} \right),$$

$$\Phi \left(\frac{z}{R} \right) = \frac{L^2}{4R^2} \sum_{j=1}^{S(z)} 1/z_j \,_1F_1 \left(\frac{3}{2}, 2, -2\pi^2 z_j R^2/L^2\right).$$

For small correlation radii $NR^2 \ll 1$, all the terms in Eq. (19) are of the same order, the hypergeometric function $\,_1F_1 \left((2n-1)/2, n, -2\pi^2 z_j R^2/L^2\right) \sim \,_1F_1 \left((2n-1)/2, n, 0\right) = 1$, and Eqs. (19) can be simplified as

$$\frac{z_j^{1/2} L^2}{R^2} = -\frac{1}{2} \chi_j \left(4j^4 + 6z_j j^2 + \frac{5}{2} z_j^2\right) - 2\chi_j \sum_{j'} S(z) \left(1 - \delta_{jj'}\right) j'^2 j^{2}$$

(23)

Then
correlations. In this sense, the interlevel transitions are more important for the short-range length to the correlation radius of surface inhomogeneities, \(2 \pi \zeta S \ll 1\), the contribution of this highest level will recover the form indicated by (25).

With the appearance of a new level \(S\) even for large \(2 \pi \zeta S \gg 1\), the contribution of this highest level will recover the form indicated by (25). Only later, when the hypergeometric function will become

\[
\Phi \left( z, \frac{R}{L} \right) = \frac{\pi^{7/2} R}{2^{1/2} L} \sum_{j=1}^{S(z)} \left( \frac{\nu(z) - j^2}{j^4} \right)^{5/2}
\]

(25)

Note that Eq. (25) for large \(NR^2\) can be improved near the critical values of \(z\) which correspond to changes in number of occupied levels \(S\). With the appearance of a new level \(S\), the number of particles on this level, \(z_S\), and, therefore, \(z_S R^2/L^2\) are small even for large \(R/L\), and the contribution of this level is \(z_S/1F_1 \left( \frac{3}{2}, 2, -2\pi^2 z_S R^2/L^2 \right) \sim z_S\), and not \(z_S \pi^{1/2} \left( 2\pi^2 z_S R^2/L^2 \right)^{3/2}\) as it is implied by Eq. (25). Only later, when the hypergeometric function will become small, \(2\pi^2 z_S R^2/L^2 \gg 1\), the contribution of this highest level will recover the form indicated by (25).

The argument of the exponents and hypergeometric functions can be also written as the ratio of the particle wavelength to the correlation radius of surface inhomogeneities, \(2\pi z_S R^2/L^2 \sim (R/\lambda_j)^2\). Therefore, as it was mentioned in the Introduction, the particle wavelength serves as a natural scale for describing the correlations and separates long-range from short-range correlations. In this sense, the interlevel transitions are more important for the short-range correlations.

The diffusion coefficient is related to the mobility (24) as

\[
D_{yy} = D_{zz} = -\sigma_{yy}/e^2 \sum_j \int \frac{\partial n_j}{\partial \epsilon} \frac{m d\epsilon}{\hbar^2} = \frac{\hbar^2}{e^2 m} \sigma_{yy} = \frac{L^2 \hbar}{\pi^3 mL^2} \Phi \left( z, \frac{R}{L} \right),
\]

while the mean free path along the channel is

\[
\mathcal{L} = \sigma \langle q > /e^2 N = (2\pi)^{1/2} \hbar \sigma \left( \sum N_j^2 \right)^{1/2} /e^2 N^{3/2}
\]

(27)

IV. TRANSPORT ALONG FILMS AND CHANNELS: HIGH TEMPERATURES

At finite temperatures all the levels with different \(j\) are populated. As a result, the transport equation becomes an infinite set of coupled equations. The chemical potential is the same for particles on all levels,

\[
\mu(N, T) = \frac{1}{2m} \left( \frac{\pi j \hbar}{L} \right)^2 + \mu_j(N_j, T), \quad \epsilon_j(q) = \frac{1}{2m} \left( \frac{\pi j \hbar}{L} \right)^2 + q^2
\]

(28)

where \(\mu_j\) is the chemical potential of a 2D system of \(N_j\) fermions on level \(j\). If we are dealing with a dilute gas, then \(\mu_j\) depends only on the number of particles on the corresponding level \(z_j = 2N_j L^2 / \pi\),

\[
z_j = \vartheta_T \ln \left( 1 + \exp \left( \frac{\mu_j}{T} \right) \right) = \vartheta_T \ln \left( 1 + \exp \left( \frac{\mu}{T} - \frac{j^2}{\vartheta_T} \right) \right),
\]

and

\[
\mu_j = T \ln \left( \exp \left( \frac{z_j}{\vartheta_T} \right) - 1 \right)
\]

(29)

where

\[
\vartheta_T = \frac{2mTL^2}{\pi^2 \hbar^2}
\]

describes the ratio of the temperature to the energy of zero-point oscillations in the well of the width \(L\). This equation should be used to express the chemical potential via the total number of particles \(z = 2NL^2 / \pi\),

8
\[ z = \vartheta T \sum_{j=1}^{\infty} \ln \left[ \exp \left( \frac{\mu}{T} - \frac{j^2}{\vartheta T} \right) + 1 \right] \]  

The solution of this equation \( \mu(z) \) at \( T = 0 \) is given by Eq. (13).

In this Section we will calculate transport coefficients for particles with Boltzmann distribution function. In the case of high-temperature Boltzmann systems,

\[ z \sim \vartheta T \exp \left( \frac{\mu}{T} \right) \Theta, \quad \mu = T \ln \left( \frac{z}{\vartheta T \Theta} \right), \quad \Theta(\vartheta T) = \sum_{j=1}^{\infty} \exp \left( -\frac{j^2}{\vartheta T} \right) \]

and the transport equation (4) in dimensionless variables \( \chi_j \),

\[ n_j(q) = n_j^{(0)}(q) \left( 1 - \frac{F L^3}{\pi^4 T^2} \chi_j \cos \theta \right) \]

assumes the form

\[
u^{1/2} = \frac{1}{2\pi^2 L^2 \ell^2} \left\{ \chi_j(q) \left[ \frac{1}{4} u^2 (\eta_1(u, u) - \eta_0(u, u)) + u j^2 (\gamma_1(u, u) - \gamma_0(u, u)) + \right. \right. \\
+ \sum_{j' \neq j} j'^2 j'^2 [\chi_{j'} \gamma_1(u, u) - \chi_j \gamma_0(u, u)] \left. \right\} \]

while the mobility (conductivity) is

\[ \sigma_{yy} = \sigma_{zz} = \sum_{j=1}^{\infty} \sigma_{yy}^{(j)} = -\frac{e^2 L^2}{2\pi^4 h^2 \vartheta T} \int \sum_{j=1}^{\infty} \exp \left( -\frac{j^2}{\vartheta T} \right) \int u^{1/2} \chi_j(q) \exp \left[ -\frac{u}{\vartheta T} \right] \, du \]

Here

\[ u = q^2 \left( \frac{L}{\pi \hbar} \right)^2, \quad S(u, j) = \text{Int} \left[ (u + j^2)^{1/2} \right], \quad u_{j,j'} = u + j^2 - j'^2, \]

and \( \gamma_i, \eta_i, \) and \( \gamma_i \) are the corresponding angular Fourier harmonics of the functions

\[ \zeta(q - q') = \zeta (q^2 + q'^2 - 2qq' \cos \varphi), \quad \eta(q - q') = \zeta(q - q') [1 - \cos \varphi]^2, \]

\[ \gamma(q - q') = \zeta(q - q') [1 - \cos \varphi] \]

over the angle \( \varphi \). In essence, the variable \( u = (qL/\pi \hbar)^2 \) plays the same role as the Fermi momenta \( z_j = \left( q_j^{(j)} L/\pi \hbar \right)^2 \) for degenerate systems in the previous Section.

In the Gaussian case (3), integration in (31) leads, of course, to the same set of equations (13) with the only difference that \( z_i \) should be substituted by \( u \). The situation is again non-analytic since the summation in (33) for off-diagonal transitions over \( j' \) should be performed up to the value \( S(u, j) \) which is not only different for each \( j \), i.e., for each equation, but also depends on momentum \( q \) and exhibits step-like jumps at certain values of \( u = q^2 (L/\pi \hbar)^2 \). However, this non-analyticity manifests itself more noticeably in the integrands (32) rather than in transport coefficients themselves which are fairly smooth. Finally, the conductivity (mobility) is equal to

\[
\sigma_{yy} = \sum_{j=1}^{\infty} \sigma_{yy}^{(j)} = \frac{e^2 NL^4}{\pi^5 \hbar L^2} \Pi \left( \frac{\vartheta T}{L} \right),
\]

\[ \Pi(x,y) = \frac{1}{x^2 \Theta(x) y^2} \sum_{j=1}^{\infty} \int \chi_j(u) \exp \left( -\frac{j^2 + u^2}{x} \right) \, du \]

Function \( \Pi(\vartheta T) \) is plotted in Fig. 4 \( (R/L = 0.05) \) and Fig. 5 \( (R/L = 0.5; 1) \).
In the Boltzmann temperature range, the diffusion coefficient can be expressed via mobility as

$$D_{yy,zz} = -\sigma_{yy}/e^2 \sum_j \int \frac{\partial n_j}{\partial \epsilon} \frac{m \, d\epsilon}{\pi \hbar^2} = \frac{T \sigma_{yy}}{e^2 N} \frac{TL^4}{\pi^5 \hbar \ell^2} \Pi \left( \frac{\vartheta_T}{T}, \frac{R}{L} \right),$$

(35)

while the mean free path

$$\mathcal{L} = \sigma \langle q \rangle /e^2 N = \frac{(mT)^{1/2} L^4}{\pi^5 \hbar \ell^2} \Pi \left( \frac{\vartheta_T}{T}, \frac{R}{L} \right)$$

(36)

The difference between the functions $\Pi(x)$ in Figs.4,5 by several orders of magnitude is not surprising. Since $x = \vartheta_T \sim (L/\lambda)^2$ ($\lambda$ is the particle wavelength), Fig.4 is potted in the region $L \sim \lambda$. On the other hand, $y = R/L = 0.05$ is rather small meaning that $R/\lambda \ll 1$. As it was explained in I (and is confirmed by the present calculation), condition $R/\lambda \ll 1$ corresponds to nearly specular quantum reflection, and, therefore, to large particle mean free paths. Thus the large values of $\Pi(x)$ in Fig.4. In Fig.5, $y = R/L \sim R/\lambda \sim 1$. This case corresponds to the most effective scattering of particles by surface inhomogeneities and to the smallest values of the mean free path.
V. SUMMARY AND DISCUSSION

In summary, we calculated mobility and diffusion coefficients for ballistic particles in ultra-narrow channels and films with random rough boundaries in conditions when the motion of particles across the films is quantized. We obtained explicit expressions for transport coefficients via the correlation function of surface inhomogeneities. The most important consequence of a discrete character of the particle spectrum for the motion across the film is the non-analytic low-temperature dependence of the transport coefficients on the film thickness and the density of particles.

The form of this non-analyticity strongly depends on the correlation radius of surface inhomogeneities $R$. In the case of short-range correlations of surface inhomogeneities, the low-temperature dependence of transport coefficients on particle density and film thickness has a pronounced saw-like structure. The saw teeth become smaller and the saw-like structure gradually disappears with increasing correlation radius. Finally, for long-range correlations one gets only not very well pronounced kinks, instead of the saw teeth, at critical values of density and/or thickness at which the number of occupied levels changes by one.

Though both the amplitude and the correlation radius of surface inhomogeneities affect the particle scattering by the walls, the dependence of transport coefficients on the amplitude of the surface inhomogeneities $\ell$, in contrast to their dependence on the correlation radius $R$, is quite trivial, and reduces to a multiplicative factor $\ell^{-2}$.

In general, the non-analytic nature of the curves is explained by the singularities in low-temperature distribution of degenerate fermions over a system of discrete energy levels. However, the sharp discontinuities on the saw-like curves for transport coefficients are caused not by the singularities in the density of state, but mostly by the interlevel transitions caused by the scattering on random rough walls. The beginning of the occupation of a new level leads to two transport effects: to the direct transport contribution of the particles from this new level, and to the opening of new scattering channels for particles on all already occupied levels (interlevel transitions to and from the new level). The first effect is proportional to the number of particles on the new level and is small. For this reason the non-analyticity of the transport coefficients reduces, in the absence of interlevel transitions, to a series of kinks corresponding to the appearance of the new levels. On the other hand, the opening of new scattering channels with the interlevel transitions to and from newly occupied levels affects particles on all already occupied levels thus increasing dramatically the total effective scattering cross-section in a step-like manner. If one artificially freezes these transitions, the transport curves will exhibit kinks rather than the saw teeth. Not surprisingly, the contribution of interlevel transitions depends exponentially on the ratio of the particle wavelength to the correlation radius of the surface inhomogeneities, and decreases rapidly with increasing correlation radius of surface roughness (i.e., with flattening of surface inhomogeneities).

Note, that the parameterization of transport parameters in this paper is slightly different from I. In the case of the mean free path it is, probably, better to use, instead of (27), (36), the parameterization in the form

$$L \sim \frac{L^2 R}{\ell^2} f(R/\lambda)$$

with the minimum at $R \sim \lambda$. The transformation of the results to this form is fairly obvious in both degenerate and Boltzmann regions.

VI. ACKNOWLEDGMENTS.

This work was supported by NSF grant DMR-9412769.

[1] A.E. Meyerovich, and S. Stepaniants, Phys. Rev. B 51, 17116 (1995)
[2] A.E. Meyerovich, and S. Stepaniants, Phys. Rev. Lett. 73, 316 (1994)
[3] Z. Tesanovic, M.V. Jarić, and S. Maekawa, Phys. Rev. Lett. 57, 2760 (1986)
[4] N. Trivedi, and N.W. Ashcroft, Phys. Rev. B 38, 12298 (1988)
[5] V.B. Sandomirskii, Sov. Phys.-JETP 25, 101 (1967) [Zh. Eksp. & Teor. Fiz. 52, 158 (1968)]
VII. APPENDIX. CLASSICAL AND SEMI-CLASSICAL MOTION ACROSS THE CHANNELS

In the classical limit, when the distance between levels with different $j$ becomes negligible, the above results should coincide with the results of classical calculations in Ref. I. The transition to the classical limit corresponds either to thick films and/or to the states with large quantum numbers, $j \gg 1$, when the interlevel transitions are accompanied by relatively small changes of the quantum number, $1 \sim \delta j \ll j$. The coordinate transformation (I) and the effective Hamiltonian (I) are, obviously, the same in classical and quantum cases. The matrix elements (I) of the effective bulk distortion (II) in the classical limit correspond exactly to the classical matrix elements in I. However, the classical analog of the squares of these matrix elements, and, therefore, the collision integral (II) are slightly different from Eqs. (I.17), (I.18), (I.20). The reason is that in I we used not the best approximation for the following combination of the $\delta$-functions:

$$\delta' (p_x - p'_x) \delta (p_x - p'_x) = \frac{1}{2} \left[ \delta^2 (p_x - p'_x) \right]' \simeq -\frac{L}{2\hbar} \delta' (p_x - p'_x)$$  \hspace{1cm} (37)

In classical calculations, quadratic expressions similar to (37) are not very well defined. More accurate expressions can be obtained either by working with bell-shaped functions instead of $\delta$-functions (i.e., by introducing some small dissipation in the equations), or by looking at the discrete (quantum) limit when all the combinations of the Kronecker symbols $\delta_{ik}$ are well defined. Careful analysis of the classical limit for the square of the matrix elements (I) demonstrates that in this particular case the term in the r.h.s. of Eq.(37) should be written as $-\frac{L}{2\hbar} \delta' (p_x - p'_x)$ rather than $-\frac{L}{2\hbar} \delta' (p_x - p'_x)$ and neglected in the classical limit $p_x \gg \hbar / L$ (i.e., $j \gg 1$). This leads to a more accurate classical analog of the transition probability (I),

$$W (p, p') = \frac{\zeta (q - q')}{4\pi L^2 m^2} \delta (\epsilon - \epsilon') \times $$

$$\left[ 2p_x^2 \delta (p_x - p'_x) + \frac{\Omega^2}{4} \delta'' (p_x - p'_x) \right],$$

$$\Omega (p, p') = (q - q') \cdot (p_x q + p'_x q'),$$

than Eq.(I.18).

The corresponding change in the classical collision integral does not result in any significant changes in the expressions for the classical transport coefficients. The only improvement should be the substitution of the functions

$$\frac{d \sin \theta}{\alpha + 4 \tan^2 \theta}$$

in the integrands for all transport coefficients by

$$\frac{d \sin \theta}{\alpha + 4 \beta \tan \theta + 8 \tan^2 \theta}$$

where, as in I, $\alpha (u) = (5/2) \Gamma_1 (7/2, 4, -u^2) / \Gamma_1 (3/2, 2, -u^2)$, and $\beta (u)$ is similar, $\beta (u) = (3/2) \Gamma_1 (5/2, 3, -u^2) / \Gamma_1 (3/2, 2, -u^2)$.

This change in the analytical expressions leads to more accurate results. However, numerically, the change is not very significant. This small numerical change is illustrated in Figs.6,7 for the functions $f_F (x)$ and $f_B (x)$ which describe the transport coefficients and the mean free path for Fermi and Boltzmann gases:

$$\sigma = \frac{32}{\pi^{3/2}} \frac{e^2 L^2 R^2 N}{\hbar t} x f_B (x), \quad x = \frac{h}{(4mT)^{1/2} R},$$

$$f_B (x) = x^4 \frac{\exp \left[ -x^2 z^2 / \cos^2 \theta \right]}{\Gamma_1 (3/2, 2, -z^2)} \frac{dz}{\cos^2 \theta \alpha + 4 \beta \tan \theta + 8 \tan^2 \theta},$$  \hspace{1cm} (39)

and
\[
\sigma = \sqrt{2e^2L^2} x^2 f_F(x), \quad x = \sqrt{2 \frac{p_F R}{\hbar}}
\]
\[
f_F(x) = \frac{1}{x^2} \int_{1}^{\frac{1}{x^2}} \frac{1}{_{1F_1}(3/2, 2, -x^2 \cos^2 \theta)} \cos^2 \theta \frac{1}{\alpha + 4\beta \tan^4 \theta + 8 \tan^4 \theta} \, d\sin \theta
\]

(40)

Needless to say, all the prefactors remain exactly the same as in I. The variable \(x\) describes the ratio \(\lambda/R\) in Eq.(39) and \(R/\lambda\) in Eq.(40).

FIG. 6. Function \(f_F(x)\); solid line - Eq.(39), dashed line - results I

FIG. 7. Function \(f_B(x)\); solid line - Eq.(40), dashed line - results I