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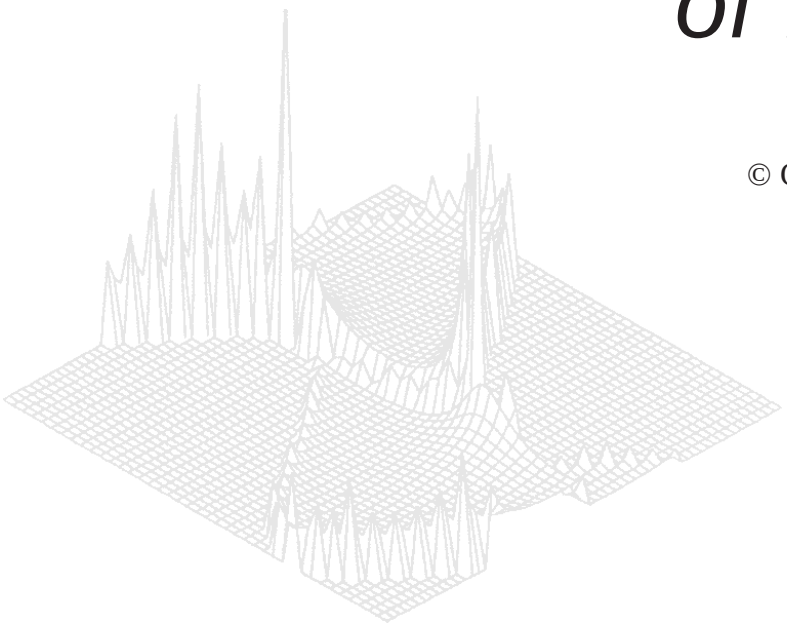

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Transport, Quantum Interference and Localisation in Ultrathin Systems with Randomly Corrugated Walls and Interfaces*

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Abstract

Comparative effects of elastic scattering by random surface inhomogeneities and bulk impurities are discussed for ultrathin quantised systems. A simple general surface collision operator is derived outside of the quantum resonance domain. Analytical and semi-analytical applications to corrugation-defined localisation and transport in various types of physical systems are presented.

1. Introduction

At first glance, the elastic scattering by random surface inhomogeneities should not be very different from scattering by bulk defects such as impurities. However, while the basic effects of impurity scattering are described in textbooks, a similar *simple* account of surface scattering is missing (see Voronovich 1994). Below we identify the processes for which the effects of weak scattering by random surface inhomogeneities and impurities are indeed similar. We derive a bulk-like surface collision operator that can be used as a general boundary condition in a wide range of parameters and apply it analytically or semi-analytically to diverse problems such as transport in ultrathin systems, bouncing ball motion, localisation of particles by corrugated substrates, multilayer systems, etc.

One always has a full set of functions that can be used as a basis for impurity problems. For randomly corrugated walls, especially with the boundary condition $\psi = 0$, the domain of existence of the wave functions and the proper basis for exact expansions are not defined. The resulting difficulties can be illustrated by the matrix element of the Hamiltonian $\widehat{H} = \widehat{H}_0 + \widehat{V}$ with the wave functions $\psi = \psi^{(0)} + \delta\psi$ (here $\widehat{H}_0$ and $\psi^{(0)}$ describe the 'flat' geometry; $\widehat{V}$ and $\delta\psi$ are the corrugation-induced changes):

$$\delta\langle\psi_1|\widehat{H}|\psi_2\rangle = \langle\psi_1^{(0)}|\widehat{V}|\psi_2^{(0)}\rangle + (E_1 - E_2)\langle\delta\psi_1|\psi_2^{(0)}\rangle\,.$$

The first term is the standard perturbative matrix element V_{12}. The second term with the corrugation-induced $\delta\psi$ is much more complicated and cannot be easily evaluated without the proper basis. This term disappears for processes

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with $E_1 = E_2$ clearing the way to an impurity-like perturbative description of boundary scattering. We will see that the corrugation-related matrix elements V_{12} calculated under the condition $E_1 = E_2$ are almost the same irrespective of particle spectra, types of walls, interfaces, and bulk fields between them.

The effect of random surface corrugation on transport and localisation of particles along random rough walls can be approached in two steps. The first one is to determine the set of physical conditions under which one can perform the perturbative calculations with $E_1 = E_2$ in the intermediate states and circumvent the difficulty caused by the lack of the proper expansion basis. After this is done, one can use the standard bulk-like transport technique similar to that for bulk impurities. The main issue is how to define the corrugation-induced part $\widehat{V}$ of the Hamiltonian unambiguously.

As the first step, the present authors have derived diagrammatically a *quantum* transport equation for systems with weak scattering by random rough walls or bulk impurities (Meyerovich and Stepaniants 1998). The essential difference from the standard Keldysh technique in combination with impurity averaging (see Rammer and Smith 1986) is the quantisation of motion in the x-direction perpendicular to the walls; the motion along the walls remains quasiclassical. This quantisation requires the replacement of the 3D bulk energy spectrum $\epsilon(\mathbf{p})$ by a set of 2D minibands $\epsilon_j(\mathbf{q})$ and results in the matrix form of the transport equation. Almost always, this quantum transport equation with weak surface or impurity scattering acquires the simple Boltzmann–Waldmann–Snider form

$$\frac{dn_j(\mathbf{q})}{dt} = 2\pi \sum_{j'} \int W_{jj'}(\mathbf{q}-\mathbf{q}')[n_{j'}(\mathbf{q}') - n_j(\mathbf{q})]\delta(\epsilon_{j\mathbf{q}} - \epsilon_{j'\mathbf{q}'}) \frac{d^2q'}{(2\pi)^2}\,, \qquad (1)$$

where $n_j(\mathbf{q})$ is the distribution function of particles in miniband $\epsilon_j(\mathbf{q})$, $\mathbf{q}$ is the 2D momentum in the direction parallel to the walls, and $W_{jj'}(\mathbf{q}-\mathbf{q}')$ is the probability of collision-induced transitions between the states $(j,\mathbf{q})$ and $(j',\mathbf{q}')$. In the range of parameters in which equation (1) is valid, the remaining problem is to relate the transition probabilities $W_{jj'}(\mathbf{q}-\mathbf{q}')$ for scattering by random rough walls to the statistical and geometrical properties of surface inhomogeneities.

Equation (1) cannot be used in a narrow quantum resonance region in which the gaps between the quantised energy levels Ω are comparable to the effective corrugation-induced transition probability, $\Omega\tau \sim 1$. Since the energy gaps Ω increase with decreasing spacing L between the walls as $1/L^2$, this presence of an anomalous quantum resonance domain is inevitable with miniaturisation of the system. The quantum resonance regime $\Omega\tau \sim 1$ corresponds to a moderately large number S of minibands $\epsilon_{j\mathbf{q}}$ accessible to a particle with energy E and is described by one of the conditions (Meyerovich and Stepaniants 1998):

$$S \sim (LR/\ell^2)^{\frac{2}{3}} > 1,\ L^2/R^2\,;$$

$$1 < S \sim (L^2/R\ell)^{\frac{2}{3}} < L^2/R^2\,, \qquad (2)$$

where ℓ and R are the average 'height' (amplitude) and 'size' (correlation radius) of surface corrugation. The second equation should be used when the correlation radius of the surface inhomogeneities is much smaller than the spacing between the

walls, $R \ll L$, and the first one should be used elsewhere. [Note that our method requires that the amplitude of the inhomogeneities ℓ should be much smaller than their correlation radius and spacing between the walls, $\ell \ll R, L$. This condition means that the inhomogeneities have small amplitude and are not sharp and that the particle phase and direction of momentum do not change much after a single collision with the wall; in the opposite case of strong roughness the mean free path $\mathcal{L} \sim L$ and the transport problem becomes trivial.] The quasiclassical range of large quantum numbers $S \gg 1$, as well as the ultra-quantum limit of small S, are outside of the quantum resonance domain (2). In the quantum resonance regime, transport processes are coupled to off-diagonal (mixed) quantum states and cannot be approximated by equation (1) which accounts only for the diagonal (pure) states. This resonance coupling makes the description of weak impurity and surface scattering becomes almost intractable.

Outside of this quantum resonance region, the coupling to the off-diagonal mixed states is small. The case $\Omega\tau \ll 1$ is effectively a single-band case, while at $\Omega\tau \gg 1$ the contribution of the off-diagonal states contains $1/\Omega\tau$ and is small. The emerging quantum transport equation for pure states with quasiclassical motion *along* the walls reduces to equation (1). As an additional benefit, equation (1) contains the energy δ-function in the collision operator and allows one to ignore the lack of the basis wave functions, at least in the second order in boundary scattering.

Below we study only the 'normal' regime (1) and show that the surface-induced transition probability W is system-independent for a wide range of systems and physical problems.

2. Corrugation-Driven Collision Operator

There are several approaches to calculation of the matrix elements of the 'corrugation-induced perturbation' $\widehat{V}$ and the corrugation-driven transition probabilities $W_{jj'}(\mathbf{q}, \mathbf{q}') = \langle |V_{j\mathbf{q},j'\mathbf{q}'}|^2 \rangle_\xi$ (here $\langle ... \rangle_\xi$ is the averaging over the random surface inhomogeneities).

One can start from the exact single-wall S-matrix (Voronovich 1994) and expand it to a multi-wall situation and particles with different spectra. Unfortunately, because of the interwall interference, the multi-wall S-matrix does not factorise into a simple product of single-wall ones. As a result, this approach is not used beyond the simplest single- or two-wall systems without interference (Makarov *et al.* 1995).

The 'adiabatic' approximation for the wave function (Kawabata 1993) can circumvent the lack of an explicit basis for wave functions in systems with randomly corrugated boundaries. If the change of the wave function along the channel with two randomly corrugated walls,

$$x = \pm L/2 \mp \xi_{1,2}(y, z), \;\; \langle \xi_{1,2} \rangle = 0 \tag{3}$$

is slow, one can start from the 'adiabatic' wave function

$$\Psi \sim \exp(iq_y y + iq_z z) \sin\left[\pi j \frac{x + L/2 - \xi_2(y,z)}{L - \xi_1(y,z) - \xi_2(y,z)}\right]. \tag{4}$$

This requires a slow variation of the wall shape along the channel, $qR \gg j, j\ell/L$ (where R is the 'size' of inhomogeneities, i.e. the correlation radius of surface corrugation). This restriction, by itself, is not perturbative and is sufficient for the calculation of the matrix elements and the reflection coefficient. However, the *transport* calculations rely on the perturbative Boltzmann equation which requires an extra condition on the smallness of the wall corrugation, $\ell \ll R, L$. In the end, the 'adiabatic' transport restrictions are equivalent to supplementing the perturbative condition $\ell \ll R, L$ by a strong extra condition $qR \gg S$ (where S is the number of occupied and/or accessible minibands). Taken together, these restrictions are stronger than the ones used in purely perturbative calculations. On the positive side, the adiabatic method, when applicable, makes the physics transparent. The adiabatic method fails in the quantum resonance regime.

The most consistent approach is the exact mapping of the problem with the corrugated boundaries onto an equivalent problem with flat boundaries and distorted bulk (Tesanovic *et al.* 1986; Trivedi and Ashcroft 1988; Meyerovich and Stepaniants 1994, 1995, 1997). For a single wall $x = x_0 + \xi(y, z)$, the flattening is a simple coordinate shift, $X = x - \xi(y, z)$. The conjugate momentum transformation, $\widehat{p}_x = \widehat{P}_x$, $\widehat{p}_{y,z} = \widehat{P}_{y,z} - \xi'_{y,z}\widehat{P}_x$ transforms the Hamiltonian $\widehat{H}_0(\mathbf{p}, \mathbf{r})$ into $\widehat{H}_0(\mathbf{P}, \mathbf{R}) + \widehat{V}(\mathbf{P}, \mathbf{R}, \xi)$ with a random bulk part $\widehat{V}$ that depends on the wall corrugation $\xi(y, z)$. With two walls with the average clearance L, $x = \pm L/2 \mp \xi_{1,2}(y, z)$, both walls can be flattened simultaneously by stretching the film, $X = [x + \xi_1/2 - \xi_2/2]/[1 - \xi_1/L - \xi_2/L]$, $Y = y$, $Z = z$. The conjugate momentum transformation $\widehat{\mathbf{p}} \to \widehat{\mathbf{P}}$ identifies explicitly the effective random bulk distortion $\widehat{V}\{\xi_{1,2}\}$. The matrix elements of $\widehat{V}$ with the wave functions ψ_0 for the flat geometry provide the transition probabilities $W_{jj'}(\mathbf{q}, \mathbf{q}')$. Though the Jacobian J of this transformation is $J \neq 1$, the Jacobian-generated terms in W are small outside the resonance region (2) and can be disregarded (for a detailed analysis of the mapping transformation approach and bibliography see Meyerovich and Stepaniants, 1998). With the same accuracy, the two-wall results can be extended to the multilayer geometry by applying the coordinate transformations to each layer independently. The mapping transformation approach provides a rigorous mathematical definition of the 'corrugation-induced' bulk-like perturbation $\widehat{V}$ and allows one to control the accuracy at each step of the calculations.

At present, the mapping transformation method is the only one that can extend the calculations to the quantum resonance region (2) though the Jacobian-generated terms make the results non-universal (system-specific) and hinder the application to multilayer systems.

The fourth and the simplest approach is to replace a wall by some potential $U(x)$ and to calculate the distortion $V = \xi\partial U/\partial x$ related to the corrugation-driven ambiguity in the wall's position, $U(x + \xi) = U_0 + \xi\partial U/\partial x$ (Fishman and Calecki 1989, 1991). This approach assumes the energy conservation in all intermediate states and cannot be used in the quantum resonance regime.

We expanded the last approach to multi-wall systems with interwall interference. Since the accuracy of this approach is unclear, the results were controlled using the more consistent mapping transformation approach. Outside of the quantum resonance regime, both approaches led to the same universal results for a wide range of systems such as:

- systems with a single random rough wall $x = \xi(y,z)$, $\langle\xi\rangle = 0$; the particles are bound to it by some attractive potential $U(x)$, $U(x \to \infty) = 0$; $U = \infty$ on the wall
- single-wall systems, $x = \xi(y,z)$, with particles confined near the wall by a holding potential, such as gravity or an electric field, with $U(x \to \infty) = \infty$
- systems with two impenetrable rough external walls, $x = \pm L/2 \mp \xi_{1,2}(y,z)$, $\langle\xi_{1,2}\rangle = 0$, with an arbitrary potential $U(x)$ in-between; $U = \infty$ on the walls
- layered systems with corrugated transparent interfaces between the layers, $x = x_\alpha + \xi_\alpha(y,z)$, and an arbitrary bulk potential $U(x)$ in-between (the potential changes abruptly by $[U]_\alpha$ on the interface); the overall confinement in the x-direction is ensured either by impenetrable external walls or by a holding potential
- particles with an arbitrary spectrum $\epsilon(\mathbf{p}) = \epsilon(-\mathbf{p})$, such as $p^2/2m$, 'relativistic' spectrum cp, spectra with gaps, etc., for these geometries.

We calculated the corrugation-induced transition probability $W_{jj'}^{\alpha\beta}(\mathbf{q},\mathbf{q}')$ between the states $\Psi_{j\mathbf{q}}^{(0)} = \psi_{j\mathbf{q}}^{(0)}(x)\exp(i\mathbf{q}\cdot\mathbf{s})$ (where $\Psi_{j\mathbf{q}}^{(0)}$ is the wave function *without* corrugation). For an interlayer interface α, the corrugation-induced perturbation is $\widehat{V}^{(\alpha)} = \xi_\alpha \partial U/\partial x = \xi_\alpha [U]_\alpha \delta(x - x_\alpha)$, and the corrugation-induced transition probabilities are

$$W_{jj'}^{\alpha\beta} = \mathrm{Re}\big[\zeta_{\alpha\beta}(\mathbf{q}-\mathbf{q}')[U]_\alpha [U]_\beta^* \psi_{j\alpha}^{*(0)} \psi_{j'\alpha}^{(0)} \psi_{j\beta}^{(0)} \psi_{j'\beta}^{*(0)}\big]\,, \tag{5}$$

where $\psi_\alpha^{(0)} = \psi^{(0)}(x = x_\alpha)$, and $\zeta(\mathbf{q})$ is the Fourier image of the correlation function of corrugation,

$$\zeta_{\alpha\beta}(\mathbf{q}) = \int d\mathbf{s}\, e^{i\mathbf{q}\cdot\mathbf{s}} \int d\mathbf{s}_1\, \xi_\alpha(\mathbf{s}_1)\xi_\beta(\mathbf{s}_1+\mathbf{s})\,.$$

The terms in W with $\alpha = \beta$ describe the transitions caused by the multiple scattering by the same wall, and the off-diagonal terms with $\alpha \neq \beta$ describe the effect of interwall correlations of surface inhomogeneities on transitions.

For impenetrable external walls with $U \to \infty$, the potential should be excluded from the matrix elements of $\xi_\alpha \partial U/\partial x$ with the help of the Schrödinger equation. In the end, the probabilities W of transitions caused by scattering by rough external walls are determined by the derivatives of unperturbed wave functions on the walls:

$$W_{jj'}^{(\alpha\beta)} = \frac{1}{4m^2}\mathrm{Re}[\zeta_{\alpha\beta}\psi_{j\alpha}^{*(0)'}\psi_{j'\alpha}^{(0)'}\psi_{j\beta}^{(0)'}\psi_{j'\beta}^{*(0)'}]\,. \tag{6}$$

The external wall (α)–interlayer interface (β) interference term in the scattering probability is

$$W_{jj'}^{(\alpha\beta)} = -\frac{1}{2m}\mathrm{Re}\big[\zeta_{\alpha\beta}[U]_\beta \psi_{j\alpha}^{*(0)'}\psi_{j'\alpha}^{(0)'}\psi_{j\beta}^{(0)}\psi_{j'\beta}^{*(0)}\big]\,. \tag{7}$$

Equation (5) for internal interfaces is the same irrespective of the particle spectrum, while equations (6) and (7) are written for $\epsilon = p^2/2m$ [general equations

for arbitrary $\epsilon(\mathbf{p})$ are too cumbersome]. For particles $\epsilon(\mathbf{p})$ in a homogeneous two-wall system, equation (6) should be replaced by

$$W_{jj'}^{(\alpha\beta)} = \frac{\zeta_{\alpha\beta} j^2 j'^2}{L^2} \frac{[\epsilon_{j\mathbf{q}'} - \epsilon_{j'\mathbf{q}}]^2}{(j^2 - j'^2)^2} \left[\delta_{\alpha\beta} - \frac{1 - \delta_{\alpha\beta}}{(-1)^{j+j'}} \right]. \tag{8}$$

Usually, the inhomogeneities from different surfaces $\alpha \neq \beta$ are not correlated with each other and $\zeta_{\alpha\beta} = 0$. If the surfaces $\alpha \neq \beta$ are correlated (Altfeder *et al.* 1998), the interwall contribution is non-trivial: while $W^{(\alpha\alpha)}$ is always positive, the sign of the interwall term $W^{(\alpha\beta)}$ with $\alpha \neq \beta$ is not fixed, and the interwall interference can be constructive or destructive depending on a particular realisation of the system; overall, W is positive since $\zeta_{\alpha\alpha}(\mathbf{q}) + \zeta_{\beta\beta}(\mathbf{q}) \geq 2|\zeta_{\alpha\beta}(\mathbf{q})|$. For example, the interwall term for a homogeneous film with two impenetrable external walls (6) is an oscillating function of the band indices,

$$W_{jj'}^{(12)} = -\frac{1}{L^2 m^2} (-1)^{j+j'} \left(\frac{\pi j}{L} \right)^2 \left(\frac{\pi j'}{L} \right)^2 \mathrm{Re}\zeta_{12}(\mathbf{q} - \mathbf{q}'). \tag{9}$$

Finally, the collision operator in equation (1) is determined by the sum of all corrugation-induced $W^{(\alpha\beta)}$ over all walls,

$$\frac{dn_j}{dt} = 2\pi \sum_{\alpha,\beta,j'} \int W_{jj'}^{(\alpha\beta)} [n_{j'} - n_j] \delta(\epsilon_{j\mathbf{q}} - \epsilon_{j'\mathbf{q}'}) \frac{d^2 q'}{(2\pi)^2}. \tag{10}$$

3. Effective Elastic Relaxation Time

The integration in the transport equation (10) over dq' is done using the energy δ-function, $\delta(\epsilon_{j\mathbf{q}} - \epsilon_{j'\mathbf{q}'}) = \delta(q' - q_{jj'})/v_{jj'}$, where $q_{jj'}$ is the solution of the equation $\epsilon_{j'}(\mathbf{q}_{jj'}) = \epsilon_j(\mathbf{q})$, and $v_{jj'} = (\partial \epsilon_{j'\mathbf{q}'}/\partial q')_{q'=q_{jj'}}$ is the velocity for isotropic $\epsilon_{j\mathbf{q}}$. The angular integration is eliminated, as usual, by using the angular harmonics. The currents are given by the first harmonic of the distribution $n_j^{(1)} \equiv \nu_j$, the equation for which involves only the zeroth and first harmonics ${}^{(0,1)}W_{jj'}(q, q_{jj''})$ of $W(\mathbf{q} - \mathbf{q}_{jj'})$ over the angle $\widehat{\mathbf{q}\mathbf{q}}_{jj'}$,

$$\begin{aligned} d\nu_j(q)/dt = & -\sum_{j'} \nu_{j'}(q_{jj'})/\tau_{jj'}, \\ \frac{2}{\tau_{jj'}} = & \sum_{\alpha,\beta,j''} \left[(\delta_{jj'}\, {}^{(0)}W_{jj''}^{(\alpha\beta)} - \delta_{j'j''}\, {}^{(1)}W_{jj'}^{(\alpha\beta)}) \frac{q_{jj''}}{v_{jj''}} \right]. \end{aligned} \tag{11}$$

This collision operator (effective relaxation time) $\widehat{\tau^{-1}}$ in equation (11) serves outside of the resonance region (2) as a general boundary condition for the diverse types of systems described above. This matrix transport equation and the relaxation time operator closely resemble those for the bulk impurity problem. The angular harmonics of the surface correlation function in the scattering probabilities (5)–(8), $\zeta^{(0)}(|\mathbf{q} - \mathbf{q}_{jj'}|) - \zeta^{(1)}(|\mathbf{q} - \mathbf{q}_{jj'}|)$, play the role of the impurity transport cross section, $\sigma_{tr}(|\mathbf{q} - \mathbf{q}_{jj'}|) = \sigma^{(0)} - \sigma^{(1)}$.

The set of S in equations (11) for the distribution functions $\nu_j(q)$ is complicated. The level of complexity depends on the number of equations S and on the range of q for which this set should be solved. The number of equations is the number of occupied or energetically accessible minibands $\epsilon_j(\mathbf{q})$ and can be very large or even infinite. In each equation, the arguments of the distribution functions ν_j and $\nu_{j'}$, q and $q_{jj'}(q)$, are different reflecting the integral nature of the collision operator. The number of equations becomes finite and involves only a finite set of the values q in two situations. For degenerate fermions, the values of q and $q_{jj'}$ in the equation for $\nu_j(q)$ are the Fermi momenta q_j and $q_{j'}$ for minibands j and j', $E_F = \epsilon_j(q_j) = \epsilon_{j'}(q_{j'})$, while the number of occupied minibands is restricted by the Fermi energy E_F. For single-particle problems, the values of q and $q_{jj'}$ are the momenta q_j and $q_{j'}$ of the particle with overall energy E in the minibands j and j', $E = \epsilon_j(q_j) = \epsilon_{j'}(q_{j'})$, while only a finite number of the minibands are energetically accessible. In other situations, e.g. for particles with the Boltzmann distribution function, the number of occupied minibands is technically infinite, while the equations should be solved for all values of q.

In three important physical situations equations (11) decouple from each other and the matrix $\tau_{jj'}^{-1}$ becomes diagonal, $\tau_{jj'}^{-1} = \tau_j^{-1}\delta_{jj'}$. Then the set (11) can be solved analytically. This happens when:

(i) only the first (lowest) quantum state j is energetically accessible, $S = j = j' = 1$ and the set (11) reduces to a single linear equation with

$$\frac{2}{\tau_{11}} = \sum_{\alpha,\beta} \left[{}^{(0)}W_{11}^{(\alpha\beta)} - {}^{(1)}W_{11}^{(\alpha\beta)} \right] \frac{q_{11}}{v_{11}} ; \tag{12}$$

(ii) the clearance between the surfaces is small, $L \ll R$, and the energy split $\Omega_{jj'} \propto 1/L^2$ between levels is large; then the interband transitions are negligible in comparison to intraband scattering, $W_{j\neq j'} \ll W_{jj}$, and

$$\frac{1}{\tau_{jj'}} \simeq \frac{1}{\tau_j}\delta_{jj'}, \quad \frac{1}{\tau_j} = \tfrac{1}{2} \sum_{\alpha,\beta} \left[{}^{(0)}W_{jj}^{(\alpha\beta)} - {}^{(1)}W_{jj}^{(\alpha\beta)} \right] \frac{q_{jj}}{v_{jj}} ; \tag{13}$$

(iii) the particle wavelength is large, $qR \ll 1$, and all W are constant with ${}^{(0)}W = 2W(0)$, ${}^{(1)}W = 0$ (quantum reflection):

$$\frac{1}{\tau_j} = \sum_{\alpha,\beta} \sum_{j'} W_{jj'}^{(\alpha\beta)}(0) \frac{q_{jj'}}{v_{jj'}} . \tag{14}$$

In all other cases, equations (11) have to be solved numerically.

4. Examples and Applications

The analytical calculations involving equations (12)–(14) can be performed for any surface correlator $\zeta(\mathbf{s})$. The correlator should be specified in numerical applications; the examples below use the most common Gaussian correlators $\zeta^{(\alpha\beta)}(\mathbf{s}) = \ell_{\alpha\beta}^2 \exp(-s^2/2R_{\alpha\beta}^2)$ with the hypergeometric angular harmonics ${}^{(0)}\zeta - {}^{(1)}\zeta = 4\pi\ell^2 R^2 {}_1F_1(\frac{3}{2},2,-2q^2R^2)$. To avoid parameter clutter, we assume that $R_{\alpha\beta}$ are the same, $R_{\alpha\beta} = R$, while the amplitudes $\ell_{\alpha\beta}$ are different, $\ell_{\alpha\beta}^2 = a_{\alpha\beta}\ell^2$ (ℓ is the scale)

The most direct application is the calculation of diffusion, conductivity, and mobility coefficients for particles in quantised films and channels with an average clearance L between the corrugated walls in the absence of external field $U(x)$. This has been done in detail in our previous paper for degenerate fermions (Meyerovich and Stepaniants 1998). That paper contains the analytical expressions for the conductivity σ, graphs of σ in different ranges of $p_F R$, R/L and S, the analysis of interwall correlations for this geometry, etc. A typical example is the conductivity of an ultrathin metal film of thickness L at $p_F R \ll 1$,

$$\sigma = (2e^2L^2/\pi^4\ell^2)\Pi(z, R/L)\,,$$

$$\Pi\left(z, \frac{R}{L}\right) = \frac{3L^2/4R^2(a_{11}+a_{22})}{S(z)(S(z)+1)(2S(z)+1)} \sum_{j=1}^{S(z)} \frac{\nu(z)-j^2}{j^2[1+\Xi_j]}\,,$$

$$\Xi_j = \frac{6}{2S(z)+1}\frac{(-1)^{j+S(z)}a_{12}}{a_{11}+a_{22}}, \quad z = \frac{2}{\pi}NL^2\,,$$

where N is the 2D density of electrons, and $\nu = (p_F L/\pi)^2$. Here Ξ_j shows that the interwall correlations cause an oscillating effect in conductivity, similar to Fig. 2 below, depending on whether the number of occupied minibands S is even or odd. The effect of interwall correlations gradually decreases with the increase in S. Though the approach used by Meyerovich and Stepaniants (1998) was less general than the one discussed above, the results are the same and need not be repeated here.

The second example is the single-particle diffusion D in quantised systems with rough walls,

$$D(L \ll R) = \frac{L^2/4\pi S\ell^2R^2}{a_{11}+a_{22}+2a_{12}} \sum_{j=1}^{S} \frac{v_j^3/j^2q_j(\partial\epsilon_{j\mathbf{q}_j}/\partial j)^2}{{}_1F_1(\frac{3}{2}, 2, -2q_j^2R^2)}\,. \tag{15}$$

This equation can be used for quasiparticles with an arbitrary energy spectrum $\epsilon(\mathbf{p})$. Examples are the single-electron diffusion in ultrathin metal films and channels or quasiparticle diffusion through capillaries or superleak in superfluid Heii.

Fig. 1 illustrates equation (15),

$$D(\omega) = \frac{L^3c}{\ell^2}\frac{1}{a_{11}+a_{22}+2a_{12}}\Pi(R/L, R\omega/c)\,, \tag{16}$$

for 'phonons' [particles with linear spectrum, $\epsilon(\mathbf{p}) = cp$] as a function of frequency $\alpha = R\omega/c$ at $R/L = 314$.

Fig. 2 shows the energy dependence of the single-particle diffusion coefficient

$$D(E) = (L^2/m\ell^2)\Pi(R/L, R\sqrt{2mE}) \tag{17}$$

for particles with quadratic spectrum, $p^2/2m$, $\alpha = R\sqrt{2mE}$, in the opposite limit $L \gg R$, for $R/L = 0{\cdot}003$, $a_{11,22} = 1$ and two interwall amplitudes $a_{12} = 0$ and $0{\cdot}7$ (solid and dotted lines).

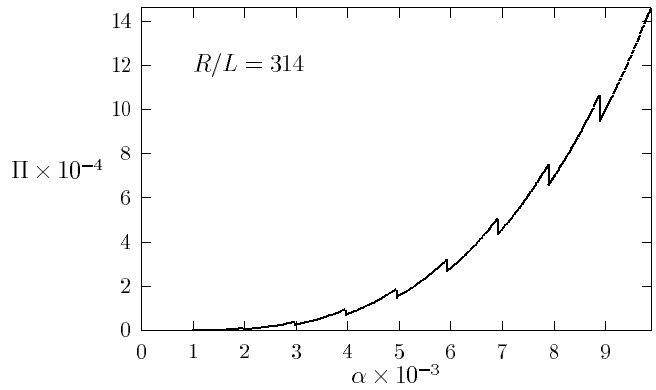

Fig. 1. The function $\Pi(\alpha)$, $\alpha = R\omega/c$, for the single-phonon diffusion coefficient (equation 16) at $R/L = 314$.

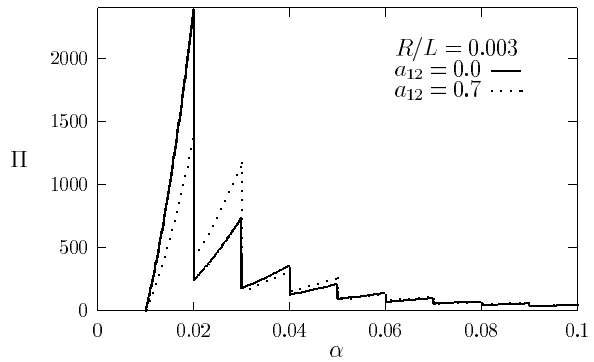

Fig. 2. Single-particle function $\Pi(\alpha)$, $\alpha = R\sqrt{2mE}$, for the single-particle diffusion coefficient (17) at $R/L = 0{\cdot}003$, with $a_{11,22} = 1$ and $a_{12} = 0$ (solid line) and $a_{12} = 0{\cdot}7$ (dotted line).

The singularities (vertical drops) in Figs 1 and 2 occur at the points in which the number S of energetically accessible minibands $\epsilon_j(\mathbf{q}) = [(\pi j/L)^2 + q^2]/2m$ increases by 1 with increasing particle energy. The reason for the drop in the mean free path and transport coefficients is the opening of additional scattering channels associated with transitions into and from this newly accessible miniband and the corresponding step-like increase in the scattering cross section (for more details see Meyerovich and Stepaniants 1997).

Next, let us consider particles near a corrugated wall in a holding field mgx such as ultra-cold neutrons in a gravitational trap (Lushchikov and Frank 1978; Alfimenkov *et al.* 1992; Geltenbort *et al.* 1998; Malik *et al.* 1999) or electrons in an electric field on the helium or hydrogen surface. The size of the first bound state is $L = (2m^2g)^{-1/3}$; the energy levels ϵ_j/mgL are given by the zeros of the Airy (wave) functions. The diffusion coefficient in the longwave limit $\alpha = R\sqrt{2mE} \ll 1$ is

$$D(\alpha \ll 1) = \frac{2}{m^4 g^2 S^2 \zeta(0)} \sum_{j=1}^{S} (E - \epsilon_j) \to \tfrac{8}{5} \frac{HL^3}{mS\zeta(0)}$$

(the last equation is quasiclassical; $H = E/mg$ is the amplitude of the particle jumps).

The value of the diffusion coefficient D determines the mean free path $\mathcal{L}$ and the localisation length $\mathcal{R}$ (Lee and Ramakrishnan 1985; McGurn and Maradudin 1984; Stepaniants *et al.* 1999):

$$\mathcal{R}(E) = \mathcal{L}(E) \exp \varphi, \quad \varphi = \pi m S(E) D(E)\,,$$

where S is the number of accessible minibands $\epsilon_{j\mathbf{q}}$. For example, if only the first miniband is occupied,

$$\varphi \equiv \pi m D = \frac{2L^6}{R^4 \ell^2} \frac{q^2 R^2}{{}_1F_1(\frac{3}{2}; 2; -2q^2R^2)} \equiv \frac{2L^6}{R^4\ell^2} \Phi(qR)\,. \tag{18}$$

The function $\Phi(x)$ is plotted in Fig. 3. Being applied to ultra-cold neutrons, equation (18) shows that the weak localisation is feasible if the neutron velocities are $v < 2$ cm s^{-1} (at present, the velocities of trapped neutrons exceed 10 cm s^{-1}). The possibility to observe localisation of electrons on helium or hydrogen surfaces is more promising. Equation (18) can be applied to any particles with a single 2D bound state $\epsilon_{0\mathbf{q}} = \epsilon_0 + q^2/2m$ on a slightly corrugated substrate. One can expect localisation for hydrogen particles bound to the surface of helium: at $T \sim 1$ K, the ripplon corrugation yields $R \sim 20$ Å, $\ell \sim 0{\cdot}8$ Å; then the coefficient in (18) is $0{\cdot}3$, and the exponent $\varphi < 12$ for particles with momenta $qR < 2$.

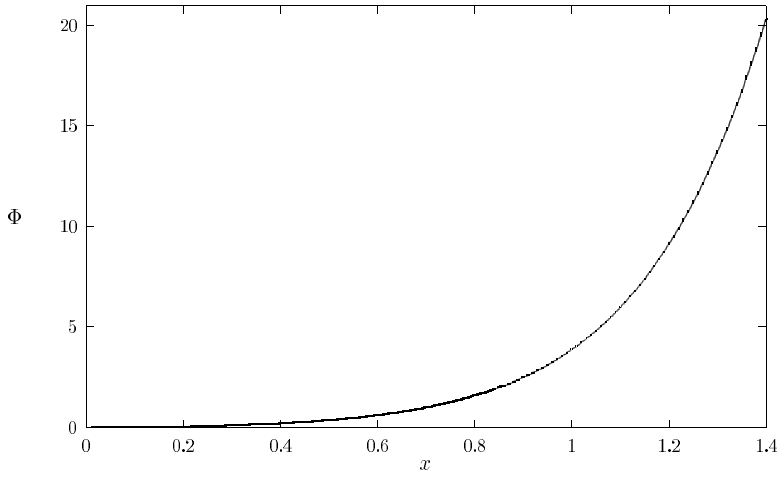

Fig. 3. The function $\Phi(x)$ (see equation 18).

5. Summary

In summary, we analysed boundary scattering effects in ultrathin ballistic systems with randomly corrugated walls. The general collision operator (11) provides a simple quantitative, often analytical, description of dissipative, transport, and localisation processes. This operator can be used, apart from the diverse examples discussed above, for transport in multilayered media in application to giant

magnetoresistance, heat transfer from trap walls to ultra-cold particles, etc. The extension to a simultaneous description of surface and bulk scattering, including the surface–bulk interference beyond the Matthiessen's rule, is straightforward.

The results provide a new insight into the difference between scattering by static and dynamic surface inhomogeneities. The latter problem arises in thermalisation between bulk and surface systems, the dynamic bouncing ball problem, scattering by surface excitations, etc. In static problems, the collision operator originates from $\langle |V_{jj'}(\mathbf{q},\mathbf{q}')|^2\rangle_\xi \delta(\epsilon_{j\mathbf{q}} - \epsilon_{j'\mathbf{q}'})$. In a non-static case, this δ-function changes to $\delta(\epsilon_{j\mathbf{q}} - \epsilon_{j'\mathbf{q}'} - \omega)$ and the *quantum* problem becomes anomalous (2) if the ratio of any pair of variables ω, Ω_{ij}, $1/\tau$ is comparable to unity. This widens the anomalous quantum regime (2) for dynamic problems.

The anomalous quantum resonance regime $\Omega_{jj'}\tau \sim 1$ given by (2) is fundamentally different. So far, it was analysed only for one- and two-wall geometries by the mapping transformation method. The description is not universal and requires system-specific calculations from the start (Meyerovich and Stepaniants 1998). For multilayer systems, both global and layer-by-layer transformations lead to singularities in the equations.

A more detailed account of the results will be published elsewhere.

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