

Rough surface scattering in many-mode conducting channels: gradient versus amplitude scattering

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We study transport properties of many-mode electron waveguides paying the main attention to the interplay between the amplitude and gradient scattering from rough surfaces. Our analysis shows that the two types of scattering are governed by different control parameters. The first (common) parameter is the ratio of the roughness amplitude to the transverse average width of a waveguide. The second parameter is determined by the squared derivative of a surface profile. We have found that the latter parameter can play the major role in the expression for the inverse mean free path, in contrast to all previous studies where the square-gradient terms were neglected. Our results may be used in experimental realizations of the surface scattering of electron waves, as well as in other applications (e.g., for optical and microwave waveguides).

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Recent numerical studies of quasi-1D disordered systems [1, 2] have revealed principal difference between surface and bulk scattering (see, e.g., discussion and references in Ref. [3]). Specifically, it was found that transport properties of quasi-1D waveguides with rough surfaces essentially depend on many characteristic lengths, in contrast to the bulk scattering where the one-parameter scaling is determined by the ratio of the localization length to the lengthwise size of samples. This fact is due to a non-isotropic character of surface scattering in the “channel space”. In particular, the transmission coefficient substantially decreases with an increase of the angle of incoming waves, see details in Refs. [2, 4]. Below we present an analytical treatment of the electron/wave scattering in waveguides with rough surfaces, focusing on the interplay between “amplitude” and “gradient” scattering mechanisms [5, 6].

Our model under consideration is a plane waveguide (or conducting quasi-1D wire) of finite width in the transverse z -direction, and infinite in the lengthwise x -direction. The lower and upper boundaries of the waveguide are defined by the equations $z = \sigma\xi_1(x)$ and $z = d + \sigma\xi_2(x)$ respectively. Therefore, the local width of the waveguide is $d(x) = d + \sigma[\xi_2(x) - \xi_1(x)]$ with the average $\langle d(x) \rangle = d$. For random functions $\xi_1(x)$ and $\xi_2(x)$ we assume $\langle \xi_1(x) \rangle = \langle \xi_2(x) \rangle = 0$ and $\langle \xi_1^2(x) \rangle = \langle \xi_2^2(x) \rangle = 1$. Thus, the parameter σ is the root-mean-square roughness height. The angular brackets stand for the average over x , or, the same, over different realizations of profiles $\xi_{1,2}(x)$. In what follows we consider three characteristic cases of rough surface profiles, which reveal generic features of the surface scattering: (A) the upper profile is rough, $\xi_2(x) = \xi(x)$, and the lower one is flat, $\xi_1(x) = 0$; (B) two rough profiles are *asymmetrical*, $\xi_1(x) = \xi_2(x) = \xi(x)$, with respect to the central line $z = d/2$; (C) two profiles are *symmetrical*,

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$-\xi_1(x) = \xi_2(x) = \xi(x)$. However, we should stress that our approach is valid for any profiles $\xi_1(x)$ and $\xi_2(x)$.

The method we use is based on the coordinate transformation,

$$x_{\text{new}} = x_{\text{old}} = x, \quad z_{\text{new}} = [z_{\text{old}} - \sigma \xi_1(x)] d/d(x), \quad (1)$$

which provides both boundaries be flat in the new variables (see, for example, Refs. [6, 7]).

(A). Let us start with the case when in old variables one surface is flat and the roughness of the other is defined by the Gaussian random function $\xi(x)$ with the binary correlator $\langle \xi(x) \xi(x') \rangle = \mathcal{W}(x - x')$. The latter is normalized to its maximal value, $\mathcal{W}(0) = 1$, and assumed to decrease on a characteristic scale R_c .

Since $\mathcal{W}(x - x')$ is an even function of its argument, the Fourier transform $W(k_x) = \int_{-\infty}^{\infty} dx \exp(-ik_x x) \mathcal{W}(x)$

is even, real and non-negative function of the lengthwise wave number k_x . One can see that the roughness power spectrum $W(k_x)$ has the maximum $W(0) \sim R_c$ at $k_x = 0$, and decreases on the scale R_c^{-1} when $|k_x|$ increases.

In order to solve the scattering problem we employ the method of the Green's function $G(x, x'; z, z')$ obeying the equation

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} + k^2 \right) G(x, x'; z, z') = \delta(x - x') \delta(z - z'), \quad (2)$$

and the Dirichlet boundary conditions $\mathcal{G}(x, x'; z = 0, z') = \mathcal{G}(x, x'; z = d(x), z') = 0$. The wave number k is equal to ω/c for a classical scalar wave of frequency ω , and is the Fermi wave number for electrons in the isotropic Fermi-liquid model.

After transformation to the new variables the equation for the canonically conjugated Green's function gets the following form (below we use the notation z instead of z_{new}),

$$\begin{aligned} & \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} + k^2 \right) \mathcal{G}(x, x'; z, z') \\ & - \left\{ \left[1 - \frac{d^2}{d^2(x)} \right] \frac{\partial^2}{\partial z^2} + \frac{\sigma \hat{U}(x)}{d(x)} \left[\frac{1}{2} + z \frac{\partial}{\partial z} \right] - \frac{\sigma^2 \xi'^2(x)}{d^2(x)} \left[\frac{3}{4} + 3z \frac{\partial}{\partial z} + z^2 \frac{\partial^2}{\partial z^2} \right] \right\} \\ & \times \mathcal{G}(x, x'; z, z') = \delta(x - x') \delta(z - z'), \end{aligned} \quad (3)$$

with flat-boundary conditions, $\mathcal{G}(x, x'; z = 0, z') = \mathcal{G}(x, x'; z = d, z') = 0$. Here the operator $\hat{U}(x)$ is defined by

$$\hat{U}(x) = \xi'(x) \frac{\partial}{\partial x} + \frac{\partial}{\partial x} \xi'(x) = \xi''(x) + 2\xi'(x) \frac{\partial}{\partial x}. \quad (4)$$

One should stress that Eq. (3) is *exact*, and valid for any profile $\xi(x)$. It contains the term (in braces) that plays the role of an effective scattering potential. Note that the potential depends not only on the profile $\xi(x)$ (resulting in the *amplitude scattering*), but also on its first and second derivatives $\xi'(x)$ and $\xi''(x)$ (the *gradient scattering*). Moreover, the last term in the scattering potential contains the square gradient $\xi'^2(x)$ giving rise to the *square-gradient scattering*. The last term is proportional to σ^2 and for this reason was neglected in all previous studies of transport properties of surface-corrugated waveguides. Below we show that in spite of its seeming smallness, this term can prevail over the others, thus, determining distinct features of the rough surface scattering. This very fact demonstrates a highly non-trivial mechanism of the surface scattering.

To proceed, we replace the boundary-value problem (3) with the equivalent Dyson-type integral equation. By assuming the smallness of the amplitude roughness, $\sigma \ll d$, this equation was averaged over the surface disorder with the use of the standard diagrammatic technique. We have to stress that in contrast to the common assumption of the smallness of σ (which allows one to use an appropriate perturbative

approach, see for example, Ref. [8]), we do not impose any restriction on the correlation length (R_c can be in arbitrary relation with σ). Our goal is the derivation of the inverse attenuation length (or, inverse mean free path) L_n^{-1} for the n -th conducting channel which is determined by the imaginary part of the proper self-energy. After quite cumbersome calculations within the second-order approximation in the perturbation potential, we have obtained the following expression,

$$\frac{1}{L_n} = \frac{1}{L_n^{(1)}} + \frac{1}{L_n^{(2)}}. \quad (5)$$

In accordance with the form of the scattering potential in Eq. (3), the inverse length L_n^{-1} is naturally presented as a sum of two terms. The first term reads as

$$\frac{1}{L_n^{(1)}} = \sigma^2 \frac{(\pi n/d)^2}{k_n d} \sum_{n'=1}^{N_d} \frac{(\pi n'/d)^2}{k_{n'} d} [W(k_n + k_{n'}) + W(k_n - k_{n'})], \quad (6)$$

where $k_n = \sqrt{k^2 - (\pi n/d)^2}$, and $N_d = [kd/\pi]$ is the total number of conducting channels (or propagating waveguide modes). Here the *diagonal term* is formed by the *amplitude mechanism* of the surface scattering (originated from the first term in the scattering potential) while the *off-diagonal terms* result from the *gradient scattering* (determined by the term containing $\sigma \xi'(x)$ and $\sigma \xi''(x)$ in Eq. (3)). The above expression (6) coincides with that obtained previously by different authors and methods (see, e.g., Ref. [8]).

The second length $L_n^{(2)}$ originates from the terms proportional to $\sigma^2 \xi'^2(x)$ in the scattering potential and therefore, belongs to the square-gradient scattering mechanism. It can be represented in the form,

$$\frac{1}{L_n^{(2)}} = \sum_{n'=1}^{N_d} \frac{1}{L_{nn'}^{(2)}} = \frac{1}{L_{nn}^{(2)}} + \sum_{n' \neq n} \frac{1}{L_{nn'}^{(2)}}. \quad (7)$$

The diagonal part,

$$\frac{1}{L_{nn}^{(2)}} = \frac{\sigma^4}{2} \frac{(\pi n/d)^4}{k_n^2} \left[\frac{1}{3} + \frac{1}{(2\pi n)^2} \right]^2 [T(2k_n) + T(0)], \quad (8)$$

with $T(k_x) = \int_{-\infty}^{\infty} dx \exp(-ik_x x) \mathcal{W}''^2(x)$ controls the electron/wave scattering *inside* the n -th channel (*intramode scattering*). The off-diagonal partial length $L_{n \neq n'}^{(2)}$, describing the *intermode scattering* from the n -th channel to $n' \neq n$ -th one, is

$$\frac{1}{L_{n \neq n'}^{(2)}} = \frac{8\sigma^4}{\pi^4} \frac{(\pi n/d)^2}{k_n} \frac{(\pi n'/d)^2}{k_{n'}} \frac{(n^2 + n'^2)^2}{(n^2 - n'^2)^4} [T(k_n + k_{n'}) + T(k_n - k_{n'})]. \quad (9)$$

To the best of our knowledge, the second term, $1/L_n^{(2)}$, in Eq. (5), is typically missed in the literature, probably, due to its seeming smallness in comparison with the first term. However, as we demonstrate below, in spite of the fact that $1/L_n^{(2)}$ is proportional to σ^4 , this term can be larger than the term $1/L_n^{(1)}$ even in the small roughness regime $\sigma \ll d$. This happens because the two lengths, $L_n^{(1)}$ and $L_n^{(2)}$, differently depend on R_c since they are determined by different independent functions, the roughness-height power spectrum $W(k_x)$ and the square-gradient power spectrum $T(k_x)$.

In Fig. 1 we display the dependence of the dimensionless quantities $A_n/2L_n^{(1)}$ and $A_n/2L_n^{(2)}$ as a function of the dimensionless correlation parameter kR_c , where $A_n = 2k_n d/(n\pi d)$ is the distance between two successive reflections of the n -th mode from the rough surface. In our numerical study we assume the random surface profile $\xi(x)$ to have the Gaussian binary correlator $\mathcal{W}(x) = \exp(-x^2/2R_c^2)$.

One can see that each pair of curves with the same channel index n intersect at some point. Specifically, for our parameters the curves with $n = 5$ intersect at the crossing point $(kR_c)_{cr} \sim 0.25$, further intersections occur at $(kR_c)_{cr} \sim 0.5, 0.75$ for $n = 20, 40$ respectively. Note that the smaller channel index n the

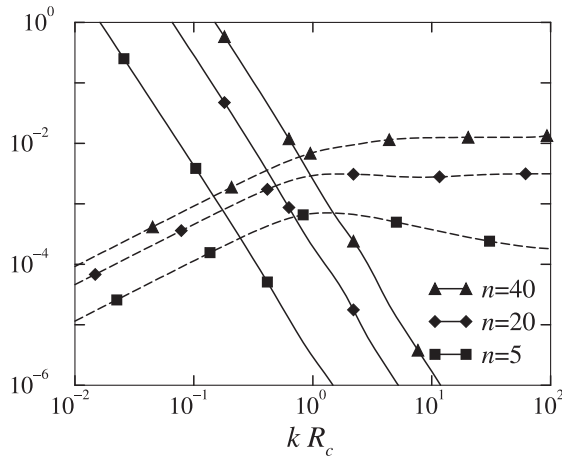


Fig. 1 $A_n/2L_n^{(1)}$ (dashed lines) and $A_n/2L_n^{(2)}$ (solid lines) versus kR_c at $kd/\pi = 50.5$, $(k\sigma)^2 = 10^{-2}$ and different values of the subchannel index n .

smaller value of the crossing point $(kR_c)_{cr}$. Since the total inverse length is given by the sum in Eq. (5), we can conclude that within the region to the left from the crossing point, the main contribution is due to square-gradient mechanism characterized by $A_n/2L_n^{(2)}$. In the second region, to the right from the crossing point, the quantity $A_n/2L_n^{(1)}$ becomes dominating.

It is noteworthy that all the curves in Fig. 1 satisfy the small-height condition $\sigma \ll d$ assumed from the beginning. Then, for the amplitude-dominated scattering where $A_n/2L_n^{(1)}$ mainly contributes, the average roughness slope is also small, $\sigma/R_c \ll 1$. The roughness slope remains to be small at the crossing points too, but increases to their left with a decrease of kR_c . As a result, to the left from the crossing point where the square-gradient term $A_n/2L_n^{(2)}$ prevails, the slope reaches the values of the order of unit, or even larger.

(B). For asymmetric profiles the width of a waveguide is constant, $d(x) = d$. Therefore, the scattering is due to the gradient and square-gradient terms only. Using the above approach one can obtain,

$$L_n^{-1} = \sum_{n'=1}^{N_d} L_{nn'}^{-1}. \quad (10)$$

Remarkably, in this case the diagonal and off-diagonal terms in Eq. (10) are rather different. Specifically, the diagonal term is proportional to σ^4 ,

$$\frac{1}{L_{nn}} = \frac{\sigma^4}{2} \frac{(\pi n/d)^4}{k_n^2} [T(2k_n) + T(0)], \quad (11)$$

in comparison with off-diagonal terms which are proportional to σ^2 ,

$$\frac{1}{L_{nn'}} = 4\sigma^2 \frac{(\pi n/d)^2}{k_n d} \frac{(\pi n'/d)^2}{k_{n'} d} \sin^4 \left[\frac{\pi(n-n')}{2} \right] [W(k_n + k_{n'}) + W(k_n - k_{n'})]. \quad (12)$$

From this expression one can see that due to specific symmetry of two surface profiles, transitions between channels with even values of $n - n'$ are forbidden (the corresponding partial scattering lengths diverge). Therefore, only the transitions between odd and even channels are allowed.

(C). For symmetric profiles the surface scattering is caused by the amplitude, gradient, and square-gradient mechanisms. The diagonal term in Eq. (10) has the form

$$\frac{1}{L_{nn}} = 4\sigma^2 \frac{(\pi n/d)^4}{(k_n d)^2} [W(2k_n) + W(0)] + \frac{\sigma^4}{2} \frac{(\pi n/d)^4}{k_n^2} \left[\frac{1}{3} + \frac{1}{(\pi n)^2} \right]^2 [T(2k_n) + T(0)]. \quad (13)$$

It can be shown that the term which is proportional to σ^2 , is due to the amplitude scattering, in contrast with the second one ($\propto \sigma^4$) which results from the square-gradient scattering. Note that in a single-mode waveguide with $N_d = 1$ the sum over n' in Eq. (10) contains only one term with $n' = n = 1$. In this case the backscattering length which enters into Eqs. (11) and (13) is in accordance with that obtained in Refs. [6].

The off-diagonal partial length $L_{n \neq n'}$ describing the intermode scattering, is due to the gradient and square-gradient scattering only,

$$\begin{aligned} \frac{1}{L_{n n'}} &= 4\sigma^2 \frac{(\pi n/d)^2}{k_n d} \frac{(\pi n'/d)^2}{k_{n'} d} \cos^4 \left[\frac{\pi(n-n')}{2} \right] [W(k_n + k_{n'}) + W(k_n - k_{n'})] \\ &+ \frac{32\sigma^4}{\pi^4} \frac{(\pi n/d)^2}{k_n} \frac{(\pi n'/d)^2}{k_{n'}} \frac{(n^2 + n'^2)^2}{(n^2 - n'^2)^4} \cos^4 \left[\frac{\pi(n-n')}{2} \right] [T(k_n + k_{n'}) + T(k_n - k_{n'})]. \end{aligned} \quad (14)$$

The absence of transitions between some channels arises in this case as in the case with asymmetric profiles (case (B)). However, in contrast to the case (B), now there are no transitions between the channels with odd difference $n - n'$. Thus, only transitions between even or odd channels are allowed.

In conclusion, we have studied the interplay between the amplitude and gradient scattering in quasi-1D waveguides with rough surfaces. Our results for the models with different symmetries between upper and lower profiles demonstrate a principal difference for these two mechanisms of scattering. In particular, we have discovered the importance of the square-gradient terms in the expression for the inverse mean free path. These terms are missed in previous studies of the surface scattering. We have found that at any fixed value σ of the roughness height, the scattering length $L_n^{(2)}$ can be smaller (and, therefore, predominating) than the known length $L_n^{(1)}$, provided the correlation length R_c is small enough. It is remarkable that the square-gradient mechanism prevails in a widely used region of a *small-scale boundary perturbations* $kR_c \ll 1$, where the surface roughness is typically described via the white-noise potential.

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