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Electron localization in narrow rough-bounded wires: evidence of different surface scattering mechanisms

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The conductance of ultra-quantum (single-mode) rough-bounded wires is calculated in frames of Hamilton approach. It is shown that in wires of finite length the electron transport exhibits both ballistic and localized regimes. We discriminate two fundamentally different competing mechanisms of electron scattering by edge roughness of conductor, viz. by-height (BH) and by-slope (BS) scattering. BH scattering leads to conventional dependence of the electron localization length L_{loc} on r.m.s. height s of boundary defects, $L_{loc} \propto s^{-2}$, while BS scattering gives $L_{loc} \propto s^{-4}$. The latter mechanism is more likely to dominate even for the case of small in height and mildly sloping roughness. Through this mechanism, generically localized quantum states of electrons (so called evanescent modes) manifest themselves significantly, in contrast to the case of electron scattering from bulk static inhomogeneities.

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1. Introduction

Application of semiconductor structures with extremely small cross section in modern technology and material science has generated a great variety of works on transport properties of such systems. In reality, boundaries and interfaces of nanostructures have either inherent (due to growth defects, fractures, etc.) or artificial (due to lithographic preparation) corrugations. Therefore, it is commonly believed that in pure quantum systems at low temperature the electron scattering is mainly caused by the surface and interface disorder (see, e.g., Refs. [1-10] and references therein). The electron-surface scattering gives rise to relaxation processes in multi-mode conductors [2,6,10] and is responsible for different mesoscopic and non-dissipative localization effects in narrow single-mode wires [1,3-5,7]. Moreover, it has been recently proved that ballistic (waveguiding) systems with bulk and surface disorder are not equivalent [8,9].

In this contribution we address the transport properties of quantum wires (strips) in which the electron scattering is caused by side edges' roughness. Two essentially different physical mechanisms are shown to be responsible for the electron-surface scattering. The first one is caused by fluctuations in the local height of edge roughness while the other is controlled by fluctuations in the roughness slopes. We call them the *by-height* (BH) and *by-slope* (BS) scattering mechanisms, respectively. These mechanisms do not interfere in the weak scattering limit and may well compete even in the simplest case of boundary corrugations being small in height and rather smooth. This competition leads to unconventional dependence of the electron localization length on the root-mean-square height and correlation length of the edge roughness as well as on other parameters of the problem.

In this report we revise an approach developed in our recent paper [11] and pay special attention to the most important physical conclusions that follows from our theory.

2. Problem formulation

We consider a conducting strip (two-dimensional electron waveguide) of length L and average width d with randomly rough edges, occupying in (x, z) plane the area restricted by inequalities

$$\begin{aligned} -L/2 \le x \le L/2, \\ -d/2 - x(x) \le z \le d/2 + x(x). \end{aligned} \tag{2.1}$$

Function $x(x)$ describes the side boundaries' roughness. It is assumed to be a random process with zero mean value, $<x(x)>=0$, and the binary correlator of the form

$$<x(x)x(x')>=s^2 W(x-x'). \tag{2.2}$$

The angle brackets stand for statistical averaging over realizations of $x(x)$, s is the root-mean-square (r.m.s.) height of the edge roughness, $W(x)$ is the correlation coefficient specified by the unit maximal value and the correlation radius R_c.

In general, the random deviations of the strip edges from straight lines give rise to fluctuations of the local width $w(x)$ of the strip and make its symmetry line ran-

domly bending. The equations (2.1) and (2.2) say that, for the sake of simplicity, we have chosen the model of the electron waveguide with non-fluctuating central straight line $z = 0$ and symmetrically fluctuating side boundaries. It is necessary to emphasize that results derived within such a model are qualitatively valid for the general case of arbitrary roughness of lateral boundaries.

In accordance with Eqs. (2.1) and (2.2), the local wire width $w(x)$ is expressed via the random function $x(x)$ by the formula

$$w(x) = d + 2x(x), \tag{2.3}$$

and, hence, possesses the following correlation properties,

$$< w(x) >= d, \quad < w(x)w(x') >= d^2 + 4s^2 W(x - x'). \tag{2.4}$$

In terms of the random width (2.3), the region (2.1) of the edge-disordered conducting strip is represented by

$$\begin{aligned} -L/2 \le x \le L/2, \\ -w(x)/2 \le z \le w(x)/2. \end{aligned} \tag{2.5}$$

The boundaries' defects are supposed to be small in height and mildly sloping,

$$s/d << 1, \qquad s/R_c << 1. \tag{2.6}$$

These limitations are common in the surface scattering theory based on perturbative approach [12].

From the linear response theory by Kubo, the dimensionless conductance $g(L)$ (in units of $e^2/p\hbar$) at zero temperature is represented by the expression

$$g(L) = -\frac{4}{L^2}\iint d\vec{r}\,d\vec{r}\,' \frac{\partial G(\vec{r},\vec{r}\,')}{\partial x}\frac{\partial G^*(\vec{r},\vec{r}\,')}{\partial x'}. \tag{2.7}$$

Here $G(\vec{r},\vec{r}\,')$ is the retarded one-electron Green function; integration over $\vec{r} = \{x, z\}$ runs over the area (2.5) occupied by the edge-irregular electron waveguide.

Within the isotropic Fermi liquid model, the function $G(\vec{r},\vec{r}\,')$ is governed by the equation

$$(\Delta + k_F^2 + i0)\, G(\vec{r},\vec{r}\,') = d(\vec{r} - \vec{r}\,'). \tag{2.8}$$

Here k_F is the electron Fermi wave number. As to the boundary conditions to equation (2.8), in the direction of current (x-axis) the conductor is regarded as open whereas in the transverse direction (z-axis) the zero (Dirichlet) conditions are applied at the true rough (symmetrical) edges of the strip, $z = \pm w(x)/2$,

$$G(\vec{r},\vec{r}\,')|_{z=\pm w(x)/2} = 0. \tag{2.9}$$

3. Mode representation

In order to separate properly the BH and BS electron-edge scattering mechanisms it is suitable to solve our problem with the use of a discrete, local in the lengthwise coordinate x, representation of normal waveguide modes, which is valid for any realization of the rough edges. To this end we perform Fourier transformation in the coordinate z using the complete set of eigenfunctions $S_n(z|x)$ of the "transverse" Laplacian, which obey the exact boundary conditions (2.9),

$$S_n(z|x) = \left[\frac{2}{w(x)}\right]^{1/2} \sin\left[\left(\frac{z}{w(x)} + \frac{1}{2}\right)pn\right], \quad n \in \aleph. \tag{3.1}$$

By substituting the Green function $G(\vec{r},\vec{r}\,')$ in the form of a double Fourier series,

$$G(\vec{r},\vec{r}\,') = \sum_{n,n'=1}^{\infty} S_n(z|x) G_{nn'}(x,x') S_{n'}(z'|x'), \tag{3.2}$$

into equation (2.8) we arrive at the following set of equations for the mode Green functions $G_{nn'}(x,x')$,

$$\left\{\frac{\partial^2}{\partial x^2} + k_F^2 - \left(\frac{pn}{w(x)}\right)^2 - \left(\frac{x'(x)}{d}\right)^2\left[1 + \frac{(pn)^2}{3}\right]\right\} G_{nn'}(x,x')$$

$$+ \frac{4}{d}\sum_{\substack{m=1 \\ (m\neq n)}}^{\infty} B_{nm}\hat{U}_x(x) G_{mn'}(x,x') = d_{nn'}d(x - x'). \tag{3.3}$$

The numerical coefficients B_{nm} and the differential operator $\hat{U}_x(x)$ are

$$B_{nm} = \frac{nm}{n^2 - m^2}\cos^2\left[\frac{p}{2}(n - m)\right], \tag{3.4}$$

$$\hat{U}_x(x) = x'(x)\frac{\partial}{\partial x} + \frac{\partial}{\partial x}x'(x). \tag{3.5}$$

The conductance expression (2.7), on substituting there Green function (3.2) and integrating over coordinates z and z', is reduced to the form

$$g(L) = -\frac{4}{L^2}\int dx dx' \sum_{n,n'=1}^{N} \frac{\partial G_{nn'}(x,x')}{\partial x}\frac{\partial G^*_{nn'}(x,x')}{\partial x'}. \tag{3.6}$$

Here $N = [k_F d/p]$ is the number of "open conducting channels", i.e. extended (propagating) waveguide modes.

Certainly, we have taken into account the conditions (2.6) of small (in height and slope) edge irregularities when deducing the mode equations (3.3) and (3.6).

Equation (3.3) for the mode Green function contains the effective electron-surface scattering potential, which consists of two (substantially different in their physical meaning) types of terms. The first term, $[pn/w(x)]^2$, is determined by random local deviation of the waveguide boundaries and, therefore, is responsible for the *by-height* (BH) scattering. All the other terms contain the gradients of

the edge roughness, $x'(x)$. Consequently, they describe the *by-slope* (BS) electron scattering. Below we will see how these two different electron-edge scattering mechanisms contribute to the effect of electron localization.

4. Single-mode wire

Keeping in mind the relevance of a surface scattering to the Anderson localization, we consider a single-mode strip where only one waveguide mode with $n=1$ can propagate. All other modes are evanescent. Therefore, the average width d is confined within the interval

$$1 < k_F d / p < 2 . \qquad (4.1)$$

Under restriction (4.1), the only element of the mode Green function matrix $\{G_{nn'}\}$ whose contribution to the conductance (3.6) at weak scattering is not parametrically small is the *intra-mode* propagator $G_{11}(x,x')$,

$$g(L) = -\frac{4}{L^2}\int dx dx' \frac{\partial G_{11}(x,x')}{\partial x}\frac{\partial G_{11}^{*}(x,x')}{\partial x'} . \qquad (4.2)$$

So, we should derive a closed equation for G_{11}. The first step of this procedure is setting $n = n' = 1$ in Eq. (3.3),

$$\left[\frac{\partial^2}{\partial x^2} + k_1^2 - V_h(x) - V_s(x)\right] G_{11}(x,x') - \sum_{m=2}^{\infty} \hat{U}_{1m}(x) G_{m1}(x,x') = d(x-x') . \qquad (4.3)$$

Here we have introduced the notation k_1^2 for the unperturbed lengthwise energy of the propagating mode ($n=1$),

$$k_1^2 = k_F^2 - \left\langle \frac{p^2}{w^2(x)} \right\rangle - \left(1+\frac{p^2}{3}\right)\frac{< x'^2(x) >}{d^2} \approx k_F^2 - (p/d)^2 . \qquad (4.4)$$

The quantities $V_h(x)$ and $V_s(x)$ are the effective *intra-mode* potentials, which are responsible for the BH and BS edge scattering, respectively. They have the form

$$V_h(x) = \frac{p^2}{w^2(x)} - \left\langle \frac{p^2}{w^2(x)} \right\rangle \approx -\frac{4p^2}{d^3} x(x) , \qquad (4.5a)$$

$$V_s(x) = \left(1+\frac{p^2}{3}\right)\frac{x'^2(x) - < x'^2(x) >}{d^2} . \qquad (4.5b)$$

In order to develop the consistent perturbative approach with respect to these potentials, we have designed them to be zero-mean-valued, i.e. $< V_{h,s}(x) > = 0$. As to the *inter-mode* BS operator potential,

$$\hat{U}_{1m}(x) = -\frac{4}{d} B_{1m} \hat{U}_x(x) , \qquad (4.6)$$

it possesses this property by definition.

Although the mode Green functions in Eq. (4.3) depend on a single space variable x, the equation (4.3) cannot be thought of as one-dimensional because of coupling the propagator $G_{11}(x,x')$ to all the inter-mode Green functions $G_{m1}(x,x')$ with mode indices $m \neq 1$. In order to obtain the closed equation for the single-mode Green function $G_{11}(x,x')$ let us rewrite the equation (3.3) for inter-mode Green function $G_{m1}(x,x')$. It can be easily shown that in the first order of approximation in the edge scattering potentials the required equation looks like

$$\left(\frac{\partial^2}{\partial x^2} + k_m^2\right) G_{m1}(x,x') = \hat{U}_{m1}(x) G_{11}(x,x') . \qquad (4.7)$$

It is substantial that, due to the single-mode condition (4.1), the wave number k_m, which specifies $G_{m1}(x,x')$, is purely imaginary, $k_m = i\,|k_m|$,

$$|k_m| = [(p\,m/d)^2 - k_F^2]^{1/2} > 0 .$$

With the use of the Green theorem one can easily derive the solution of Eq. (4.7) in the form

$$G_{m1}(x,x') = \int dx_1 G_m^{(0)}(x,x_1) \hat{U}_{m1}(x_1) G_{11}(x_1,x') . \qquad (4.8)$$

This relation contains the unperturbed Green functions $G_m^{(0)}(x,x')$, which belong to the class of *evanescent* functions. They are strongly localized in x direction,

$$G_m^{(0)}(x,x') = -\frac{\exp(-|k_m||x-x'|)}{2|k_m|} . \qquad (4.9)$$

By substituting Eq. (4.8) into Eq. (4.3), we arrive eventually at the required *closed* equation for the intra-mode propagator $G_{11}(x,x')$,

$$\left[\frac{\partial^2}{\partial x^2} + k_1^2 - V_h(x) - V_s(x)\right] G_{11}(x,x') - \int dx_1 \hat{K}(x,x_1) G_{11}(x_1,x') = d(x-x') . \qquad (4.10)$$

The kernel of the integro-differential operator entering this equation is described by

$$\hat{K}(x,x') = -\left(\frac{4}{d}\right)^2 \sum_{m=2}^{\infty} B_{1m}^2 \left[\hat{U}_x(x) G_m^{(0)}(x,x') \hat{U}_x(x') - < \hat{U}_x(x) G_m^{(0)}(x,x') \hat{U}_x(x') > \right] . \qquad (4.11)$$

Similar to the intra-mode potentials $V_{h,s}(x)$, the operator potential $\hat{K}(x,x')$ is constructed in such a way as to make $<\hat{K}(x,x')>=0$.

Equation (4.10) contains complete information on scattering of the single propagating electron mode with $n=1$ from the roughness of the conductor boundaries. The local potentials $V_h(x)$ and $V_s(x)$ are responsible for the intra-mode BH and BS scattering. The integral operator $\hat{K}(x,x')$ governs the BS intra-mode scattering but through inter-mode transitions via the evanescent modes with $n\geq 2$. From Eqs. (4.5b) and (4.11) it follows that these transitions contribute to the electron-edge scattering as much, in order of magnitude, as the direct BS scattering described by the local potential $V_s(x)$.

5. Average conductance and its moments. BH and BS backscattering length

The equation (4.10) for the single-mode Green function $G_{11}(x,x')$ is strictly one-dimensional one. Inhomogeneities of the wire edges now enter the scattering potentials rather than the boundary conditions. The Hamiltonian of the corresponding one-dimensional dynamic system is hermitian. Therefore, in order to solve the equation (4.10) and obtain the averaged conductance (4.2) we can employ one of the methods commonly used in the transport theory of one-dimensional disordered systems: the perturbative diagrammatic method by Berezinski [13,14], the invariant imbedding method [15,16], or the two-scale approach [7,11,17], which seems to be more general. Below we briefly report the results of the calculations.

The n-th moment of the dimensionless conductance is described by the relatively simple (as well as suitable for analysis) formula,

$$<g^n(L)>=\frac{4}{\sqrt{p}}\left(\frac{L_b}{L}\right)^{3/2}\exp\left(-\frac{L}{4L_b}\right)\int_0^\infty\frac{zdz}{\cosh^{2n-1}z}$$
$$\times\exp\left(-z^2\frac{L_b}{L}\right)\int_0^z dy\cosh^{2(n-1)}y,\qquad n=0,\pm1,\pm2,.... \tag{5.1}$$

The result (5.1) completely determines main averaged characteristics of the electron transport in a single-mode conducting strip. Since the conductance itself is not a self-averaged quantity, we have also calculated its self-averaged logarithm,

$$<\ln g(L)>=-L/L_b\ , \tag{5.2}$$

which displays the exponential fall of the conductance with increasing length L at the so-called representative (non-resonant) realizations of the random potential [18].

In fact, the relations (5.1) and (5.2) are common and well known in the transport theory of one-dimensional disordered systems. Our achievement lies in the backscattering length L_b, which enters these relations and gives complete information about the electron transport through the surface-disordered waveguide. This length is contributed by both BH and BS scattering potentials in Eq. (4.10). In calculating L_b, it should be taken into account that the correlation between by-height potential (4.5a) and by-slope potentials (4.5b), (4.11) must be disregarded because fluctuations of height $x(x)$ and slope $x'(x)$ are uncorrelated in the weak scattering limit [12]. Therefore, the BH and BS scattering mechanisms contribute additively to the inverse backscattering length,

$$1/L_b=1/L_b^{(s)}+1/L_b^{(h)}, \tag{5.3}$$

The expression for the inverse backscattering length $1/L_b^{(s)}$ associated with BS scattering potentials (4.5b) and (4.11) is

$$\frac{1}{L_b^{(s)}}=\frac{1}{2k_1^2}\left(\frac{s}{d}\right)^4\int_{-\infty}^{\infty}\frac{dq}{2p}(q^2-k_1^2)^2\tilde{W}(q-k_1)\tilde{W}(q+k_1)$$
$$\times\left[\left(1+\frac{p^2}{3}\right)+4(q^2-k_1^2)\sum_{m=2}^{\infty}B_{1m}^2\,\tilde{G}_m^{(0)}(q)\right]^2. \tag{5.4}$$

The backscattering length $L_b^{(h)}$ related to the BH scattering potential (4.5a) is described by

$$\frac{1}{L_b^{(h)}}=\frac{4p^4s^2}{k_1^2d^6}\tilde{W}(2k_1). \tag{5.5}$$

The functions $\tilde{W}(q)$ and $\tilde{G}_m^{(0)}(q)$ are the Fourier transforms of the correlation function $W(x)$ from (2.2) and the evanescent Green function (4.9), respectively.

6. Discussion

1. With the aid of the general formula (5.1) we can write down the expressions for average resistance $<g^{-1}(L)>$ and average conductance $<g(L)>$ of the edge-disordered single-mode wire.

The average resistance. At $n=-1$ the integrals in Eq. (5.1) are calculated exactly. So we get

$$<g^{-1}(L)>=\frac{1}{2}\left[1+\exp\left(\frac{2L}{L_b}\right)\right]. \tag{6.1}$$

The average conductance. At $n=1$ the integration in Eq. (5.1) can be performed asymptotically in the parameter L/L_b. This gives the following results,

$$<g(L)>\approx 1-L/L_b\ ,\qquad L\ll L_b\ ; \tag{6.2a}$$

$$< g(L) >\approx \frac{p^{5/2}}{2}\left(\frac{L}{L_b}\right)^{-3/2}\exp\left(-\frac{L}{4L_b}\right), L >> L_b . \quad (6.2b)$$

The expressions for the average resistance (6.1) and conductance (6.2) as well as the expressions for all their moments (5.1) are entirely consistent with the localization theory for one-dimensional disordered systems. Specifically,

(i) In short wires, when $L << L_b$, the average conductance exhibits the ballistic behavior, $< g(L) >\approx 1$.

(ii) The diffusive (metallic) regime of the electron transport is not present at any length of the wire.

(iii) On the contrary, in long wires with $L >> L_b$, the resistance (6.1) displays an exponential increase with increasing strip length L, while the conductance (6.2b) shows an exponential decrease as the length L exceeds the value of $4L_b$. Such behavior of transport characteristics is typical for conduction electrons undergoing Anderson localization in one-dimensional systems. Therefore, the quantity $L_{loc} \equiv 4L_b$ is conventionally called the (one-dimensional) localization length.

2. The formulae (5.1), (5.2), and hence (6.1), (6.2), are universal and applicable for any one-dimensional degenerate system subject to weak static disorder. The physical nature of the disorder determines only the backscattering lengths L_b. We have found that *surface disorder* is characterized by two scattering mechanisms. Both BH and BS surface scattering mechanisms contribute independently to the electron backscattering length L_b. To make the correct comparison of the BH scattering length (5.5) and the BS length (5.4) we give their asymptotic for the Gaussian correlation function of roughness, $W(x) = \exp(-x^2 / R_c^2)$.

(i) The BH length $L_b^{(h)}$ demonstrates the conventional dependence on the statistical parameters of the disordered edges, s and R_c, as well as on the average strip width d and the electron wave number k_1 [3,4],

$$R_c / L_b^{(h)} \sim (s / d)^2 (R_c / d)^4 \exp(-k_1^2 R_c^2) / (k_1 R_c)^2 . \quad (6.3)$$

In particular, the inverse BH backscattering length is quadratic in the roughness r.m.s. height s.

(ii) The inverse length of the BS backscattering shows the unexpected dependence on the parameters of the problem,

$$\frac{R_c}{L_b^{(s)}} \sim \left(\frac{s}{R_c}\right)^4 \left(\frac{R_c}{d}\right)^2 \qquad \text{for} \qquad R_c << d , \quad (6.4a)$$

$$\frac{R_c}{L_b^{(s)}} \sim (k_1 s)^4 \left(\frac{R_c}{d}\right)^2 \exp\left(-\frac{k_1^2 R_c^2}{2}\right) \text{ for } R_c >> d . \quad (6.4b)$$

(iii) It is evident from the expressions (6.3) and (6.4) that the ratio $L_b^{(h)} / L_b^{(s)}$ is the product of a small parameter and a large one. So, the BH and BS backscattering lengths can arbitrarily relate to each other, and their ratio is highly sensitive to the statistical properties of the rough edges. If the BS scattering prevails, then the inverse backscattering length is proportional to the fourth power of the roughness r.m.s. height, $1/L_b^{(s)} \propto s^4$. All these features should be taken into account when analyzing experimental data.

3. A remarkable peculiarity of BS scattering mechanism is that through this scattering the evanescent modes manifest unexpectedly their significance, though they are strongly localized in the direction of propagation and normally do not directly contribute to the energy transport in waveguide systems. In the problem considered here, the evanescent modes determine the kernel (4.11) of the operator potential in Eq. (4.10). This potential can be seen to govern intra-mode scattering of the single propagating mode with $n = 1$ through inter-mode transitions via the virtual evanescent modes with $n \geq 2$. Those transitions contribute to the expression (5.4) for the BS backscattering length as much, in order of magnitude, as the direct BS scattering governed by the potential (4.5b). It should be emphasized that contribution of the evanescent modes to the kinetic coefficients of the propagating mode seems to be a distinctive feature of the scattering in surface-corrugated waveguide systems. This is not the case for waveguides with weak bulk disorder [19].

4. As far as we know, until the present time there has not been made any reasonable distinction between BH and BS scattering in surface-disordered systems. Only the existence in general of different competing mechanisms responsible for wave scattering from rough surfaces was indicated in Ref. [20] on the basis of the experimental results. The relative function of these mechanisms in dynamic processes of waveguide-like systems was not properly analyzed.

In this work, the method has been suggested within the framework of which both of the above-mentioned scattering mechanisms appear quite naturally, being associated with different terms of the Hamiltonian. We have demonstrated that at least in a single-mode waveguide the scattering caused even by mildly sloping boundary defects can be attributed to either *by-height* or *by-slope* scattering mechanism, depending on the statistical properties of the roughness. It is noteworthy that taking into account the BS mechanism is particularly essential if boundary roughness is classified as being large-scale ($k_1 R_c >> 1$).

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