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Correlated roughness effects on electrical conductivity of quantum wires

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The influence of electron scattering by rough boundaries on electrical conductivity of quantum wires is studied in the diffuse transport limit within the kinetic Boltzmann equation approach. The considerations are restricted to the wires obtained by lateral confinement of a two-dimensional electron gas. Both intra- and interboundary roughness correlations are taken into account. It is shown that the cross correlations usually increase the conductivity, leaving the shape and phase of the quantum size oscillations almost unaffected. © *2001 American Institute of Physics.*
[DOI: 10.1063/1.1372656]

I. INTRODUCTION

Progress in nanofabrication technology in recent years has made it possible to impose lateral confining potential on a two-dimensional electron system, and to produce quasione-dimensional quantum wires. Laterally confined quantum structures have been fabricated, for instance, in GaAs/AlGaAs heterostructures, where the split-gate or etching techniques allow the lateral modulation of the composition and the band gap.[1] In such structures, long mean free path of charge carriers in comparison with the wire width leads to transport phenomena due to nonlocal effects[2,3] and to some anomalies in the low-field Hall effect.[4] Apart from this, scanning probe microscopy techniques enabled production of nanowires of Al,[5] Fe,[6] and Co[7] with a wire width smaller than 10 nm.

It has been shown experimentally that electron scattering from rough boundaries has a strong influence on the magnetoresistance of long wires, and in general on their transport properties.[8] In fact, if the wire width is comparable to the Fermi wavelength, pronounced quantum-size-effect (QSE) oscillations with the wire width are expected. This has been shown, e.g., in Ref. 9, where magnetotransport in quantum wires in the presence of scattering from rough boundaries was studied. The roughness was described there in terms of a Gaussian correlation function by two parameters—the root mean square (rms) roughness amplitude Δ and the lateral correlation length ξ. It was shown that the roughness scattering leads to a large positive magnetoresistance for wire widths larger than the Fermi wavelength λ_F and correlation lengths smaller than λ_F. Boundary roughness in quantum

wires was also shown to have a significant influence on the current distribution and Hall effect.[10] In some other studies of single and coupled quantum wires in a magnetic field,[11] the boundary roughness was considered only in terms of the Gaussian correlation function.

Quantum-mechanical calculations of electrical conductivity have also been performed for quantum wires with a wide range of boundary morphologies. In that case, some additional features arise from possible boundary fractality, described by the roughness exponent H.[12–16] The boundary fractality was shown to have a significant influence on wire conductivity. The considerations, however, were limited to incoherent electron scattering from different boundaries, neglecting this way effects arising from possible cross correlations between the wire boundaries. This problem is analyzed in the present article in which we include cross correlations and analyze their influence on electrical transport properties.

The article is organized as follows. In Sec. II we present general expressions for electrical conductivity of quantum wires. Model boundary roughness is described in Sec. III. Numerical results are presented and discussed in Sec. IV. Final conclusions and some general remarks are in Sec. V.

II. CONDUCTIVITY OF QUANTUM WIRES

We consider a two-dimensional (2D) electron gas, confined laterally by an external potential to form a long quantum wire. The axis x is along the wire and the axis y is perpendicular to the wire but within its plane (the plane of the 2D electron gas). The wire boundaries are located at $y_1 = y_1^0 + h_1(x) \equiv -d/2 + h_1(x)$ and $y_2 = y_2^0 + h_2(x) \equiv d/2 + h_2(x)$, where d is the wire width and $h_1(x)$ and $h_2(x)$ are two random functions, average values of which vanish by definition, $\langle h_1(x) \rangle = \langle h_2(x) \rangle = 0$. We assume that the roughness is isotropic, so that the height–height correlation func-

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tions depend only on the relative distance $|x-x'|$. We will consider the situation when the dominant contribution to electrical resistivity comes from the electron scattering due to roughness of the lateral confining potential, neglecting other sources of scattering like impurities or roughness of the vertical confining potential. Assuming step-like lateral confining potentials one may write the relevant Hamiltonian in the form[12]

$$H = \left\{ -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V_1\Theta(-y-d/2) + V_2\Theta(y\right.$$

$$\left. -d/2)\right\} + \{V_1 h_1(x)\delta(y+d/2) - V_2 h_2(x)\delta(y-d/2)\}$$

$$\equiv H_0 + H_{\text{scatt}}, \tag{1}$$

where m is the electron mass and V_β denotes height of the confining potential at the βth interface ($\beta=1,2$). The first part, H_0 in the formula (1) is the Hamiltonian of a wire with ideal boundaries, while H_{scatt} is a perturbation due to the boundary roughness. The wave functions and the corresponding eigenvalues of the Hamiltonian H_0 are $\Phi_{\nu k}(x,y) = L^{-1/2}e^{ikx}\varphi_\nu(y)$ and $E_{\nu k}=E_\nu+\hbar^2 k^2/2m$, respectively, where L is the wire length. Free electron motion is assumed along the wire, with the corresponding wave vector k, while the motion along the axis y is quantized with the corresponding discrete energy levels E_ν ($\nu=1,2,...$) and wave functions $\varphi_\nu(y)$ (assumed real). In the first term of Eq. (1) $\Theta(x)$ is the step function, $\Theta(x)=1$ for $x\geq 0$ and $\Theta(x)=0$ for $x<0$, whereas $\delta(x)$ in the second term is the Dirac delta function. One should note at this point that in real situations the lateral confining potential is not steplike, but varies with the distance from the middle of the wire in a more complex way. This general case, however, will not be considered in this article.

The wire conductivity, calculated in the Born approximation, is given by the following formula:

$$\sigma = \frac{e^2}{\hbar}\frac{\hbar^4}{8\pi^3 m^2 d}\sum_{\nu=1}^{N}\sum_{\nu'=1}^{N} k_\nu k_{\nu'}[D^{-1}(E_F)]_{\nu\nu'}, \tag{2}$$

where the matrix elements $[D(E_F)]_{\nu\nu'}$ are calculated at the Fermi energy E_F and are given by

$$[D(E_F)]_{\nu\nu'} = [D^{\text{in}}(E_F)]_{\nu\nu'} + [D^{\text{cros}}(E_F)]_{\nu\nu'}, \tag{3}$$

with

$$[D^{\text{in}}(E_F)]_{\nu\nu'} = \sum_{\beta=1}^{2}\left\{\delta_{\nu\nu'}\sum_{\mu=1}^{N} A_\nu^\beta A_\mu^\beta \frac{k_\nu}{K_\mu}[C_\beta(k_\nu-k_\mu)\right.$$

$$+ C_\beta(k_\nu k_\mu)] - A_\nu^\beta A_{\nu'}^\beta[C_\beta(k_\nu-k_{\nu'})$$

$$\left. - C_\beta(k_\nu+k_{\nu'})]\right\}, \tag{4}$$

$$[D^{\text{cros}}(E_F)]_{\nu\nu'} = -2\left\{\delta_{\nu\nu'}\sum_{\mu=1}^{N} A_\nu^{\text{cros}} A_\mu^{\text{cros}}\frac{k_\nu}{k_\mu}[C_{12}(k_\nu\right.$$

$$- k_\mu) + C_{12}(k_\nu+k_\mu)] - A_\nu^{\text{cros}} A_{\nu'}^{\text{cros}}$$

$$\left.\times[C_{12}(k_\nu-k_{\nu'}) - C_{12}(k_\nu+k_{\nu'})]\right\}. \tag{5}$$

Here, $A_\nu^\beta = V_\beta[\varphi_\nu(y_\beta^0)]^2$, $A_\nu^{\text{cros}} = \sqrt{V_1 V_2}\varphi_\nu(y_1^0)\varphi_\nu(y_2^0)$, whereas $C_\beta(k) = \int C_\beta(x)\exp(ikx)dx$ is the Fourier transform of the autocorrelation function $C_\beta(x)$, defined as $C_\beta(x) = \langle h_\beta(x)h_\beta(0)\rangle \equiv (1/L)\int h_\beta(x)h_\beta(0)dx$, for $\beta=1,2$. Since $C_\beta(x)=C_\beta(-x)$, the Fourier components are real, and $C_\beta(k)=C_\beta(-k)$. Similar definitions also hold for the cross-correlation function $C_{12}(x)$ and its Fourier components $C_{12}(k)$. The matrix elements $[D^{\text{in}}(E_F)]_{\nu\nu'}$ describe incoherent electron scattering by different boundaries, while the matrix elements $[D^{\text{cros}}(E_F)]_{\nu\nu'}$ take into account coherent scattering due to cross correlations of the wire boundaries. In the above equations N is the number of occupied one dimensional minibands, and k_ν is defined as $k_\nu=[(2m/\hbar^2)(E_F - E_\nu)]^{1/2}$.[11] The Fermi energy E_F and the number of occupied minibands N for a given wire width d and electron density n per unit area of the 2D electron gas can be determined from the condition

$$nd = \frac{2}{\pi}\left(\frac{2m}{\hbar^2}\right)^{1/2}\sum_{\nu=1}^{N}(E_F-E_\nu)^{1/2}. \tag{6}$$

When the electrons are confined by infinite potential walls ($V_\beta\rightarrow\infty$), one finds $A_\nu^\beta = \hbar^2\pi^2\nu^2/md^3$, $A_\nu^{\text{cros}} = (-1)^{\nu+1}\hbar^2\pi^2\nu^2/md^3$, and $E_\nu=(\hbar^2/2m)(\nu\pi/d)^2$.

III. WIRE BOUNDARY ROUGHNESS AND CROSS CORRELATIONS

In the following discussion we suppress the boundary index β, which will be restored at the end of this section. For a self-affine rough boundary, the height–height correlation function $C(x)=\langle h(x)h(0)\rangle$ has the scaling behavior $C(x) \approx \Delta^2 - Bx^{2H}$ if $x\ll\xi$, and $C(x)=0$ if $x\gg\xi$[13-16] with B ($\approx\Delta^2/\xi^{2H}$) being a constant. Here, ξ is the in-plane roughness correlation length, $\Delta=\langle[h(x)]^2\rangle^{1/2}$ is the saturated rms roughness amplitude, and $H(0<H<1)$ is the roughness exponent which characterises the degree of surface irregularity at small length scales ($x\ll\xi$).[13-16]

For self-affine fractals the roughness spectrum $C(k) = \int C(x)\exp(ikx)dx$ has the scaling behavior $C(k)\propto k^{-1-2H}$ if $k\xi\gg1$ and $C(k)\propto$const if $k\xi\ll1$. Such behavior can be described by the simple Lorentzian analytic model[16]

$$C(k) = \frac{\Delta^2\xi}{(1+a|k|\xi)^{1+2H}}. \tag{7}$$

Indeed, in the limit $k\xi\ll1$, we have $C(k)\approx\Delta^2\xi$, while in the limit $k\xi\gg1$ we obtain $C(k)\propto k^{-1-2H}$. The normalization condition $\int_{-k_c<k<k_c} C(k)dk=\Delta^2$ yields the constant a; $a = (1/H)[1-(1+ak_c\xi)^{-2H}]$ if $0<H<1$, and $a=2\ln(1+ak_c\xi)$ if $H=0$ (logarithmic roughness).[16] Here, $k_c=\pi/a_0$
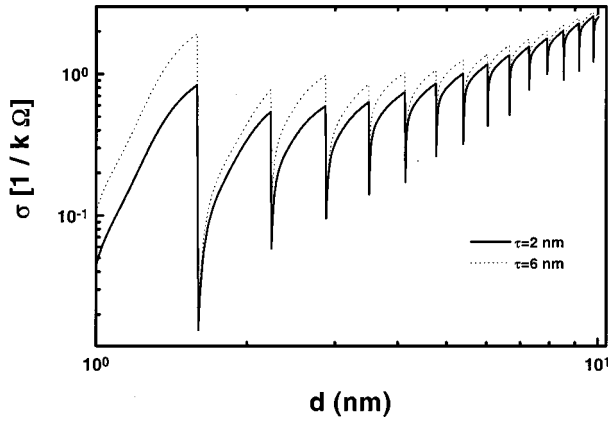
FIG. 1. Wire conductivity vs wire width d, calculated for indicated values of the decay parameter τ, $H_1 = H_2 = 0.5$, and for $\xi_1 = \xi_2 = 5$ nm.

FIG. 2. Wire conductivity vs roughness exponent ratio H_2/H_1 ($H_1 = 0.5$) calculated for indicated values of τ, $d = 5$ nm, and for $\xi_1 = \xi_2 = 5$ nm.

with a_0 being a parameter of the order of interatomic spacing. For other roughness models see also Refs. 17 and 18.

For the Fourier transform of the cross correlation function we assume for simplicity the following form:

$$C_{12}(k) = \sqrt{C_1(k)C_2(k)} \exp(-d/\tau). \tag{8}$$

This form corresponds to exponentially decaying cross correlations with increasing wire width, with the corresponding decay parameter τ. Similar forms have been used to describe real-space cross correlations in multilayer between interfaces.[19]

IV. NUMERICAL RESULTS

Numerical calculations were performed for the 2D areal electron density $n = 4.0$ nm^{-2}, atomic spacing $a_0 = 0.3$ nm, and rms roughness amplitude $\Delta_1 = \Delta_2 = 0.3$ nm, which is of the atomic dimensions. Apart from this, our calculations were performed for infinite potential walls and for the wire widths much larger than Δ_1 and Δ_2, $d \gg \Delta_1, \Delta_2$ (in order to ensure validity of the description).

Figure 1 shows electrical conductivity versus the wire width d for two different values of the decay parameter τ. As one might expect, the conductivity varies oscillatorylike with increasing d. The oscillations are of quantum origin and the corresponding oscillation period is $\lambda_F/2$ (λ_F being the Fermi wavelength). Each time the Fermi level crosses another lateral miniband, another channel for electron scattering becomes open, which reduces the conductivity and leads to the observed QSE oscillations. Since the role of boundary scattering decreases with increasing d, average magnitude of the conductivity increases with increasing wire width d. As Fig. 1 shows, the conductivity increases with increasing decay parameter τ. This is because coherent scattering due to the cross correlations reduces the contribution from the incoherent electron scattering by the wire boundaries. The shape and phase of the QSE oscillations remain almost unaffected by the cross-correlated scattering component. However, a component with the oscillation period equal to λ_F is generated by the interference term, as one can note in Fig. 1 for $\tau = 6$ nm.
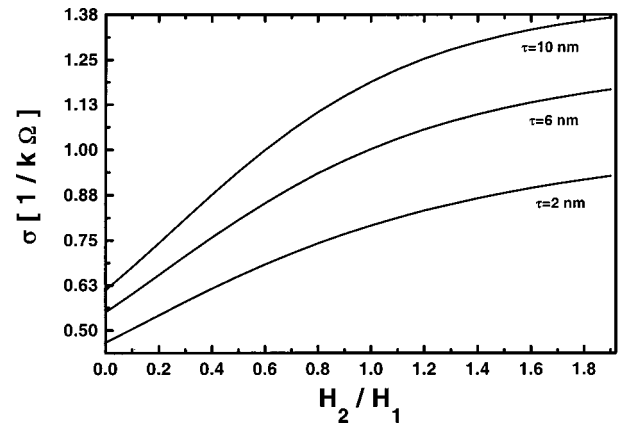
In Fig. 2 we show conductivity as a function of H_2/H_1

(at constant H_1) for several values of the decay parameter τ. As before, the conductivity increases with increasing value of τ. The conductivity also increases with increasing value of H_2/H_1, and the rate of this increase is larger for larger values of τ. Thus, boundaries with larger values of the roughness exponent H give smaller contribution to resistivity. A similar behavior is shown in Fig. 3, where the conductivity is plotted as a function H_2/H_1 (at constant H_1) for various roughness correlation lengths ξ_1 and ξ_2. At small values of H_2/H_1 and large roughness correlation lengths, $\xi_1, \xi_2 > \tau$, the conductivity increases rather fast with increasing H_2. However, when either correlation lengths or H_2/H_1 are small, the increase is significantly smaller. The conductivity also increases with increasing correlations lengths ξ_1 and ξ_2.

Variation of electronic conductivity with the roughness correlation lengths is shown explicitly in Fig. 4, where the conductivity is plotted as a function of ξ_2/ξ_1 (at constant ξ_1) and for different values of the decay parameter τ. The conductivity significantly increases in magnitude with increasing ξ_2 for $\xi_2/\xi_1 < 1$ and for large cross-correlation lengths ($\tau > d$). Similar dependence is shown in Fig. 5 for different values of the roughness exponents H_1 and H_2.
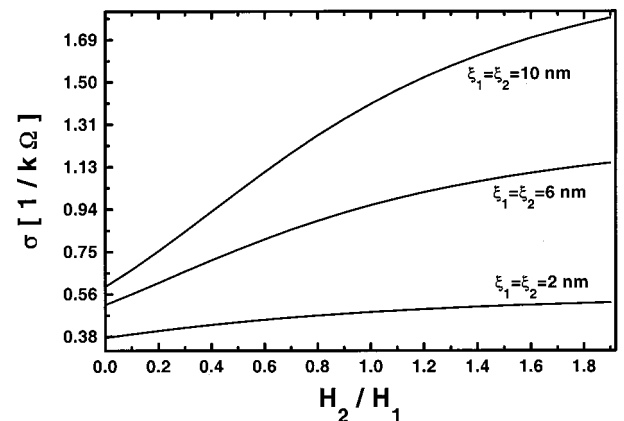

FIG. 3. Wire conductivity vs roughness exponent ratio H_2/H_1 ($H_1 = 0.5$) calculated for $\tau = 3$ nm, $d = 5$ nm, and for various boundary correlation lengths, $\xi_1 = \xi_2$.
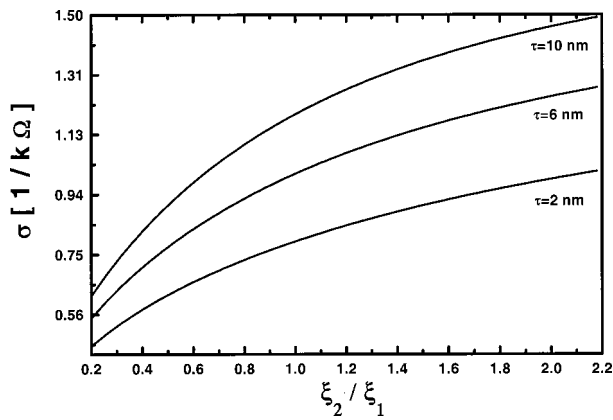
FIG. 4. Wire conductivity vs roughness correlation length ratio ξ_2/ξ_1 ($\xi_1 = 5$ nm) calculated for $d = 5$ nm, $H_1 = H_2 = 0.5$, and for indicated values of the parameter τ.
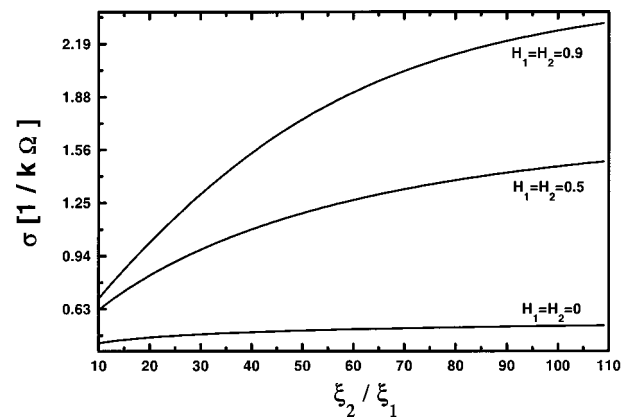

FIG. 5. Wire conductivity vs roughness correlation length ratio ξ_2/ξ_1 ($\xi_1 = 5$ nm) calculated for $\tau = 10$ nm, $d = 5$ nm, and for various values of the roughness exponents, $H_1 = H_2$.

V. CONCLUSIONS

We have analyzed the boundary scattering effects on the electrical conductivity of quantum wires formed from a 2D electron gas by lateral confinement. The lateral boundaries are described by random functions with nonzero inter- and intraboundary correlations. The formalism used to calculate the conductivity was based on the Boltzman equation, and scattering probabilities were calculated within the Born approximation. It was shown that the cross correlations leave QSE oscillations almost unaffected in shape, although the average conductivity increases in magnitude. However, an additional component with the oscillation period equal to λ_F is generated by the interference effects due to cross-correlated roughness. Moreover, it was shown that the boundary roughness correlation lengths and roughness exponents have a significant influence on the wire conductivity.

In a more realistic approach, finite confining potential and other scattering effects should be taken into account. Such effects were recently considered in the case of quantum wells, and were shown to reduce the role of electron scattering by surface/interface roughness, and consequently reduce the role of fractality effects described by the exponent H.[20] Similar behavior is expected also for one-dimensional quantum wires with self-affine rough boundaries.

ACKNOWLEDGMENTS

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