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*Published in:*
Physica Status Solidi B

*DOI:*
10.1002/(SICI)1521-3951(199902)211:2<671::AID-PSSB671>3.3.CO;2-D

phys. stat. sol. (b) **211**, 671 (1999)

Subject classification: 73.61.−r; 72.10.Fk; 73.50.Dn

# Conductivity of Quantum Wires with Rough Boundaries

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(Received July 22, 1998)

The effects due to electron scattering by rough boundaries on the electrical conductivity of quantum wires are analysed theoretically in the diffusive regime. The boundary roughness is assumed to be random self-affine fractal characterised by the roughness exponent $H$, roughness correlation length $\xi$, and rms roughness amplitude $\Delta$. In the limit of small correlation lengths and a single occupied quasi-one-dimensional miniband, the conductivity $\sigma$ shows a power-law behaviour with the wire width $d$, $\sigma \propto d^9$. For large $N$, on the other hand, the conductivity increases then as $\sigma \propto d^c$ ($c \approx 2$) with increasing $d$.

## 1. Introduction

Electron scattering by rough boundaries in confined electron systems is usually the dominant source of electrical resistance, when the size of the system is comparable to the Fermi wavelength. This takes place e.g. in ultra-thin films, where the electron gas is confined along one direction, being generally free in two others.

In quantum-mechanical calculations [1 to 3] of the electrical conductivity of thin films the boundary roughness was described by the rms roughness amplitude $\Delta$ and the correlation length $\xi$, usually in terms of Gaussian or simple exponential correlation functions. It was shown that the conductivity $\sigma$ of ultra-thin metallic films (e.g. in $CoSi_2$) [4] follows a universal power law with the film thickness $d$, $\sigma \propto d^c$ ($c \approx 2.3$) [2], while for semiconducting films a similar law with $c \approx 6$ was found [2, 5]. Both results hold in the limit $k_F\xi \ll 1$, where $k_F$ is the Fermi wavevector. In the opposite limit, $k_F\xi \gg 1$, the roughness correlation form was found to play a significant role, and the mean variation of $\sigma$ with film thickness could no longer be approximated by a power law [3]. However, one should note that the limit $k_F\xi \gg 1$ is not properly described by the Born approximation. Recently, some additional features of the roughness, that arise from possible surface/interface fractality (described by the roughness exponent $H$), were shown to have a significant influence on the film conductivity [6] and spin-valve magnetoresistance in magnetic multilayers [7].

Recent advances in nanotechnology allow to fabricate quantum wires, e.g., by imposing a lateral confining potential on two-dimensional electron gas. Such quantum structures were fabricated e.g. from GaAs/AlGaAs heterostructures. A long electron mean-free-path in comparison with the wire width leads to a wide variety of new transport phenomena in such systems, as for example bend resistance [8, 9], transfer resistance [10], or anomalies in the low-field Hall effect [11].

It has been shown experimentally that the boundary roughness scattering has a strong influence on the magnetoresistance of long wires and, in general, on their transport properties [12]. When the wire width is comparable to the Fermi wavelength, remarkable quantum size effects are also expected. Quantum-mechanical calculations of electronic transport in quantum wires with an externally applied magnetic field were performed by Akera and Ando [13] in the presence of boundary roughness scattering. The roughness was described by the rms roughness amplitude and the correlation length in terms of the Gaussian correlation function. It was shown that the roughness scattering gives rise to a large positive magnetoresistance for wire widths larger than and correlation lengths smaller than the Fermi wavelength. The boundary roughness in quantum wires was also shown to have a pronounced influence on the current distribution and Hall effect [14].

The main objective of the present paper is the analysis of fractality boundary effects in quantum wires within the formalism similar to that of Fishman and Calecki [2, 3], but reduced to one-dimensional structures. Analytical results of the wire conductivity are derived in terms of phenomenological boundary height–height correlation models for any roughness exponent $H$ in the range $0 \leq H \leq 1$. The results are compared with those obtained for two-dimensional thin films.

In Section 2 we describe briefly the theoretical formalism. The model of a rough boundary is described in Section 3. The limits of small and large numbers of occupied one-dimensional minibands are considered in Sections 4 and 5, respectively. Finally, the concluding remarks are gathered in Section 6.

## 2. Conductivity of Quantum Wires

Consider a two-dimensional electron gas in the plane $z = 0$, which is laterally confined to form a narrow quasi-one-dimensional wire along the axis $x$. The boundaries of the wire are determined by $y = -d/2 + h_-(x)$ and $y = d/2 + h_+(x)$, where the roughness is described by single-valued random functions $h_\pm(x)$. Apart from this, the roughness is assumed isotropic, so that the height–height correlation function $C_\beta(x' - x'') = \langle h_\beta(x')\, h_\beta(x'')\rangle$ $(\beta = +, -)$ depends only on the relative distance $|x' - x''|$. Denoting the potential heights outside the wire as $V_-$ for $y < -d/2 + h_-(x)$ and as $V_+$ for $y > d/2 + h_+(x)$, the system can be described by the Hamiltonian

$$H = \left\{ -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V_-\Theta(y + d/2) + V_+\Theta(y - d/2) \right\} + \{V_- h_-(x)\,\Theta(y + d/2) - V_+ h_+(x)\,\Theta(y - d/2)\} \equiv H_0 + U\,, \tag{1}$$

where $\Theta(x) = 1$ for $x \geq 0$ and $\Theta(x) = 0$ for $x < 0$. The first term, $H_0$, describes electron motion in a quantum wire with ideal boundaries. The corresponding eigenfunctions $\Phi_{\nu k}(x, y)$ and eigenenergies $E_{\nu k}$ are then given by $\Phi_{\nu k}(x, y) = L^{-1/2}\, \mathrm{e}^{ikx}\, \varphi_\nu(y)$ and $E_{\nu k} = \varepsilon_\nu + \hbar^2 k^2/2m$, respectively, where $L$ is the wire length, $\varphi_\nu(y)$ and $\varepsilon_\nu$ are the wavefunction and energy, respectively, of the $\nu$-th discrete state due to quantization of the electron motion along the $y$ direction. The second term in Eq. (1) is the scattering potential of the rough boundaries. We assumed in Eq. (1) that only the boundary morphology of the lateral confining potential contributes substantially to the electron scattering, while scattering due to nonuniformity of the potential confining electron gas to the plane $z = 0$ is neglected.

Under the assumptions described above the wire conductivity in the Born approximation is given by the formula [2, 3, 15]

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

where $N$ is the number of occupied one-dimensional minibands, whereas $k_\nu$ is defined as $k_\nu = [(2m/\hbar^2)(E_F - \varepsilon_\nu)]^{1/2}$, with $E_F$ the Fermi energy. The matrix elements $D_{\nu\nu'}$ are determined by the scattering potential $U$, and are given by

$$D_{\nu\nu'} = \sum_{\beta=+,-} \left\{ \delta_{\nu\nu'} \sum_{\mu=1}^{N} A_{\nu\beta} A_{\mu\beta} \frac{k_\nu}{k_\mu} [F_\beta(|k_\nu - k_\mu|) + F_\beta(|k_\nu + k_\mu|)] \right.$$
$$\left. - A_{\nu\beta} A_{\nu'\beta} [F_\beta(|k_\nu - k_{\nu'}|) - F_\beta(|k_\nu + k_{\nu'}|)] \right\} , \tag{3}$$

where $A_{\nu\pm} = V_\pm \varphi_\nu^2(y = \pm d/2)$, and $F_\beta(k)$ is defined as $F_\beta(k) = \langle |h_\beta(k)|^2 \rangle$. Here, $\langle |h_\beta(k)|^2 \rangle$ is the Fourier transform of the height–height correlation function $C_\beta(x)$, $C_\beta(x) = (1/L) \int \langle h_\beta(x') h_\beta(x' + x) \rangle \, dx'$. Since the boundary roughness is isotropic, one finds $\langle |h_\beta(k)|^2 \rangle = \langle |h_\beta(-k)|^2 \rangle$.

The Fermi energy $E_F$ and the number $N$ of occupied one-dimensional minibands for a given wire width $d$ and a given electron density $n$ per unit area can be determined from the condition

$$nd = \frac{2}{\pi} \left( \frac{2m}{\hbar} \right)^{1/2} \sum_{\nu=1}^{N} (E_F - \varepsilon_\nu)^{1/2} . \tag{4}$$

When the electrons are laterally confined by an infinite potential ($V_\pm \to \infty$), then $A_\nu = \hbar^2 \pi^2 \nu^2 / m d^3$ and $\varepsilon_\nu = (\hbar^2/2m)(\nu\pi/d)^2$.

## 3. Model of a Rough Boundary

For clarity of notation the boundary index $\beta$ will be suppressed in this section. For a self-affine fractal boundary the height–height correlation function $C(x)$ has the scaling behaviour $C(x) \approx \Delta^2 - B|x|^{2H}$ if $|x| \ll \xi$, and $C(x) = 0$ if $|x| \gg \xi$ [16], with $B$ being a constant ($B \approx \Delta^2/\xi^{2H}$). Here, $\xi$ is the in-plane roughness correlation length, $\Delta$ is the saturated rms surface roughness, $\Delta = \langle h(x)^2 \rangle^{1/2}$, and $H (0 \le H \le 1)$ is the roughness exponent which characterises the degree of boundary irregularity at small length scales ($x \ll \xi$) [17 to 19]. For self-affine fractals the roughness spectrum $\langle |h(k)|^2 \rangle \propto \int C(x) \, e^{-ikx} \, dx$ [16] obeys the following scaling limits:

$$\langle |h(k)|^2 \rangle \propto \begin{cases} |k|^{-1-2H} & \text{if} \quad |k|\,\xi \gg 1 , \\ \text{const} & \text{if} \quad |k|\,\xi \ll 1 . \end{cases} \tag{5}$$

The scaling behaviour given by Eq. (5) can be described by the simple Lorentzian analytic model [20]

$$\langle |h(k)|^2 \rangle = \frac{2\pi\Delta^2\xi}{(1 + a|k|\,\xi)^{1+2H}} \tag{6}$$

with $a = (1/H)[1 - (1 + ak_c\xi)^{-2H}]$ if $0 < H \le 1$, and $a = 2\ln(1 + ak_c\xi)$ if $H = 0$ (logarithmic roughness) [20]. Here $k_c$ is the cut-off vector, $k_c = \pi/a_0$, where $a_0$ is of the order

of the atomic spacing. Indeed, in the limit $|k|\,\xi \ll 1$, we have $\langle |h(k)|^2 \rangle \approx 2\pi \Delta^2 \xi$, while in the limit $|k|\,\xi \gg 1$ we obtain $\langle |h(k)|^2 \rangle \propto |k|^{-1-2H}$. Models similar to that described by Eq. (6) were also discussed in the past in the context of optical scattering from rough surfaces [21]. More complicated correlation models which are based on predictions from linear Langevin growth equations can be found for example in [22].

## 4. Limit of $N = 1$

If the wire width $d$ is sufficiently small, only a few one-dimensional minibands are occupied. When only one miniband is occupied ($N = 1$), then the conductivity reads

$$\sigma = \frac{e^2\hbar^3}{8\pi m^2 d} \frac{k_1^4}{\langle |h_-(2k_1)|^2 \rangle A_{1-}^2 + \langle |h_+(2k_1)|^2 \rangle A_{1+}^2} . \tag{7}$$

Assuming an infinite confining potential for both boundaries as well as the same amplitude $\Delta$, correlation length $\xi$ and roughness exponent $H$ one finds, on taking into account Eq. (6), the following expression for the wire conductivity:

$$\sigma = \frac{e^2 n^4}{2^9 \pi^2 \hbar} \left[ \frac{(1 + 2ak_1\xi)^{1+2H}}{\Delta^2 \xi} \right] d^9 , \tag{8}$$

where we also took into account that $k_1 = n\pi d/2$ and $A_{\nu\pm} = \hbar^2\pi^2\nu^2/md^3$ for an infinite confining potential. In the limit of small correlation lengths, $k_1\xi \ll 1$, we obtain the power law dependence of the conductivity on the wire width $d$, $\sigma \propto d^9$, which is independent of the roughness exponent $H$. In contrast, for a two-dimensional film the conductivity follows in this limit the power law $\sigma \propto d^6$ [2].

The wire conductivity as a function of the correlation length $\xi$ has a minimum at a certain value of $\xi$, which can be determined from the condition $4aHk_1\xi = 1$. Note that the parameter $a$ in this condition depends generally on $H$ and $\xi$, as described in Section 3. The minimum is clearly visible in Fig. 1, where the conductivity is shown as a

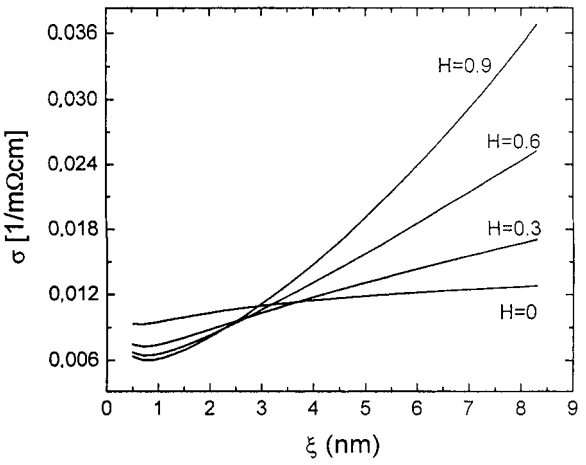


Fig. 1. Wire conductivity vs. roughness correlation length $\xi$ for the indicated roughness exponents $H$. The other parameters are:
$d = 5$ nm ($d < d_c = 9.3$ nm),
$n = 0.4\ \text{nm}^{-2}$, $a_0 = 0.3$ nm,
and $\Delta = 0.3$ nm

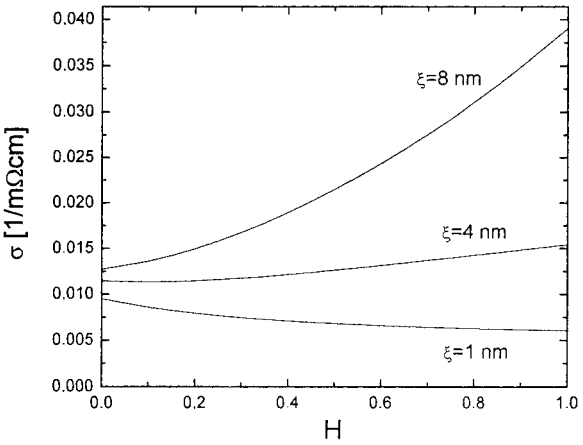


Fig. 2. Wire conductivity vs. roughness exponent $H$ for the indicated roughness correlation lengths $\xi$. The other parameters are as in Fig. 1

function of the correlation length $\xi$ for indicated roughness exponents $H$. The assumed electron density is $n = 0.4\,\mathrm{nm}^{-2}$, for which the critical wire width above which the Fermi level crosses the second one-dimensional miniband is $d_c = 9.3$ nm. For correlation lengths larger than $\lambda_F/2$ ($\lambda_F \approx 8$ nm in the case shown in Fig. 1) the conductivity increases with increasing correlation length $\xi$ and increasing roughness exponent $H$. For $\xi$ smaller than $\lambda_F/2$ the conductivity variation with $\xi$ and $H$ is more complex and the minimum becomes weaker as the roughness exponent $H$ decreases. Similar behaviour of the electrical conductivity was also found in the case of two-dimensional ultrathin films [5, 6], where the minimum, however, was more pronounced. Variation of the electrical conductivity with increasing $H$ is shown explicitly in Fig. 2. For small correlation lengths ($\xi < \lambda_F/4$) the conductivity decreases monotonously with increasing $H$, while for larger correlation lengths ($\xi > \lambda_F/2$) it monotonously increases with increasing $H$.

## 5. General Case, $N > 1$

Assume as before symmetrical wire boundaries, that is the same confining potential on both sides ($A_{\nu+} = A_{\nu-} \equiv A_\nu$) and the same roughness parameters $\Delta$, $\xi$ and $H$. For arbitrary number $N$ of occupied one-dimensional minibands the conductivity is then given by Eq. (2), with the matrix elements $D_{\nu\nu'}$ of the form

$$D_{\nu\nu'} = 4\pi\Delta^2\xi\left\{\delta_{\nu\nu'}\sum_{\mu=1}^{N} A_\nu A_\mu \frac{k_\nu}{k_\mu}\left[\frac{1}{(1+a\,|k_\nu - k_\mu|\,\xi)^{1+2H}} + \frac{1}{(1+a\,|k_\nu + k_\mu|\,\xi)^{1+2H}}\right]\right.$$
$$\left. - A_\nu A_{\nu'}\left[\frac{1}{(1+a\,|k_\nu - k_{\nu'})^{1+2H}} - \frac{1}{(1+a\,|k_\nu + k_{\nu'}|\,\xi)^{1+2H}}\right]\right\}. \qquad (9)$$

In the limit of small correlation lengths the matrix $D_{\nu\nu'}$ is approximately diagonal, $D_{\nu\nu'} \approx 8\pi\Delta^2\xi\sum_{\mu=1}^{N} A_\nu A_\mu (k_\nu/k_\mu)\,\delta_{\nu\nu'}$. Thus, in that limit the conductivity is given by the

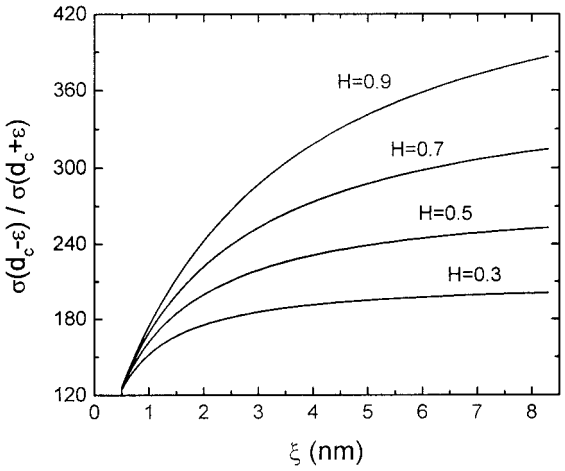


Fig. 3. Mobility ratio, $\sigma(d_c-\varepsilon)/\sigma(d_c+\varepsilon)$, vs. $\xi$ for the roughness exponents as indicated. The other parameters are: $d_c = 9.3$ nm, $a_0 = 0.3$ nm, $\Delta = 0.3$ nm, and $\varepsilon = 0.1$ nm

simplified formula

$$\sigma \approx \frac{e^2\hbar^3}{32\pi^2 m^2 d} \sum_{\nu=1}^{N} \frac{k_\nu^3}{A_\nu \Delta^2 \xi \sum_{\mu=1}^{N} (A_\mu/k_\mu)} . \tag{10}$$

In the case of two-dimensional quantum wells, an important quantity that characterises scattering processes and electronic structure is the so-called conductivity (or mobility) ratio, i.e., the ratio of conductivities (or mobilities) for the Fermi levels slightly below and above the second miniband edge [3]. A similar ratio can also be introduced in the case of quantum wires. In principle such a ratio can be measured by varying the wire width. In Fig. 3 we show the conductivity ratio as a function of the correlation length $\xi$, calculated for an infinite confining potential and for the indicated roughness exponents $H$. The ratio increases monotonously with increasing correlation length and roughness exponent $H$, contrary to the case of two-dimensional films, where the ratio

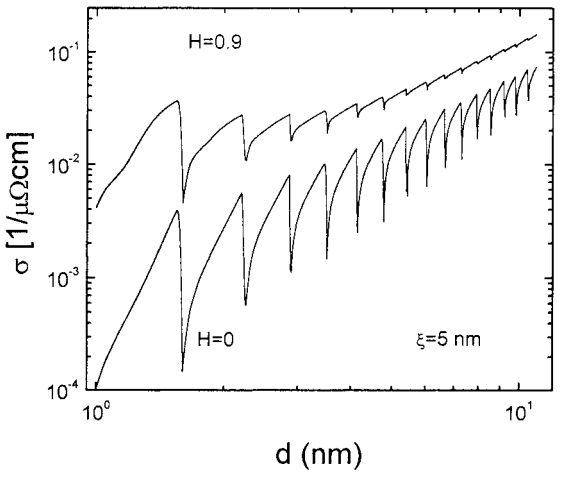


Fig. 4. Conductivity vs. wire width $d$ for $\xi$ and $H$ as indicated. The other parameters are: $n = 4\,\mathrm{nm}^{-2}$, $a_0 = 0.3$ nm, and $\Delta = 0.3$ nm

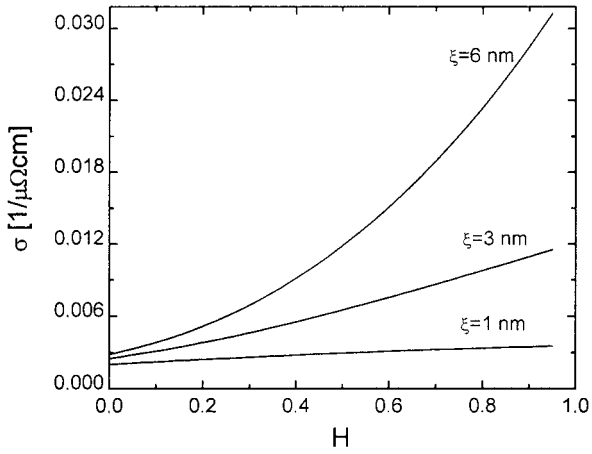


Fig. 5. Conductivity vs. $H$ for indicated roughness correlation lengths $\xi$. The other parameters are: $d = 2$ nm, $n = 4\,\mathrm{nm}^{-2}$, $a_0 = 0.3$ nm, and $\Delta = 0.3$ nm

has an extremum at a certain $\xi$. It is also worth noting that the mobility ratio in quantum wires is significantly larger than the corresponding ratio in ultrathin films.

For on infinite confining potential one finds $A_\nu \propto d^{-3}$, and the conductivity on average increases with the wire width as $\sigma \propto d^5 f(d)$, where $f(d)$ is determined by the dependence of the wave vectors $k_\nu$ on the wire width $d$. Numerical fits in the regime of the wire width $d \in (1, 10)$ nm, small correlation length ($\xi \approx 0.5$ nm) and relatively high electron density $n$ (in order to have large $N$) showed that $f(d) \propto d^{-c}$, or alternatively $\sigma \propto d^{5-c}$, with $c \approx 3$. Thus, for large $N$ the conductivity shows a similar mean variation with the wire width $d$ as in two-dimensional films in the same large $N$ limit.

The conductivity as a function of the wire width $d$ shows oscillations due to the quantum size effects. The corresponding oscillation period is equal to half the Fermi wavelength. Fig. 4 shows this behaviour for two different values of the roughness exponent $H$ and for a fixed correlation length $\xi$. The relative amplitude of the oscillations increases with decreasing $H$.

The roughness amplitude $\Delta$ has a rather trivial influence on the conductivity; namely $\sigma \propto \Delta^{-2}$ (since $\langle |h(k)|^2 \rangle \propto \Delta^2$). A significantly more complex behaviour appears when considering the dependence on the roughness exponent $H$ and correlation length $\xi$. The conductivity increases rather fast with increasing roughness exponent $H$ in the regime or large $H(\approx 1)$ and long correlation lengths, as shown in Fig. 5. It is also worth noting that for large correlation length ($k_F \xi > 1$), the conductivity can change by an order of magnitude when the roughness exponent $H$ varies from $H = 0$ to $H = 1$.

## 6. Summary

In this paper we investigated the boundary roughness scattering effects on the electrical conductivity of quantum wires formed from a laterally confined two-dimensional electron gas. The boundary roughness was assumed to be random self-affine fractal (power-law roughness) with analytic roughness spectrum characterised by the roughness exponent $H$, roughness correlation length $\xi$, and roughness amplitude $\Delta$. For the sake of simplicity and to single out the effects due to fractality, we assumed a rectangular lateral confining potential.

For quantum wires with only a single one-dimensional miniband occupied, we found a complex dependence of the conductivity on the roughness exponent $H$ and correlation length $\xi$, especially in the regime of correlation lengths comparable to half the Fermi wavelength. However, in the limit $k_F\xi \ll 1$ the conductivity follows the power law $\sigma \propto d^9$ with increasing $d$, which is independent of the roughness exponent.

For quantum wires with a large number $N$ of occupied minibands the conductivity increases as $H$ increases and/or the ratio $\Delta/\xi$ decreases (boundary smoothing). In the limit $k_F\xi \ll 1$ we found the $\sigma \propto d^2$ power law. For large correlation lengths ($k_F\xi > 1$), the conductivity is very sensitive to $H$ and can change by an order of magnitude when $H$ varies from $H = 0$ to $H = 1$.

We also showed that the conductivity ratio (or mobility ratio) for the Fermi level just above and below the second lateral miniband is significantly larger in the case of quantum wires than in the case of thin films. Moreover, the quantum size effects appear more pronounced in quantum wires, than in two-dimensional metallic films.

***Acknowledgements*** G. P. would like to acknowledge useful discussions with L. J. Geerligs. J. B. acknowledges support through the research Project 2 P03B 075 14 of the Polish Research Committee.

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