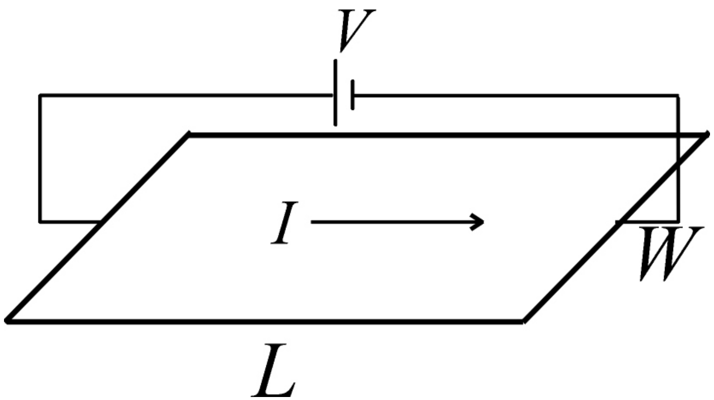
Quantum and Boltzmann transport in the quasi-one-dimensional wire with rough edges

Juraj Feilhauer and M. Mosko

Institute of Electrical Engineering, Slovak Academy of Sciences

Mesoscopic Q1D wire



A wire made of the normal metal is called *mesoscopic* if the wire length L is smaller than the electron coherence length L_ϕ [1-3] where for example:

in Au: L_ϕ (T = 40 mK) = 12 µm,

in Al: L_ϕ (T = 3 K) = 3.6 µm.

The wire is called *quasi-one-dimensional* (Q1D), if L is much larger than the width (W) and thickness (H) of the wire [3]. Fabrication of the Q1D wires from such metals like Au, Ag, Cu, etc., usually involves techniques like the electron beam lithography, lift-off, and metal evaporation. These techniques always provide wires with disorder due to *the grain boundaries, impurity atoms and rough wire edges* [4]. Disorder scatters the conduction electrons and limits the electron mean free path (l) in the wires to ~ 10 - 100nm. Of fundamental interest are the wires with W and H as small as ~ 10 - 100nm.

Objective

In work [5] we study electron transport in Q1D metallic wires made of a two-dimensional (2D) conductor ($H \to 0$) of width W and length L >> W. Our aim is to compare an impurity-free wire with rough edges with a smooth wire with impurity disorder. We calculate the electron transmission through the wires by the scattering-matrix method, and we find the Landauer conductance for a large ensemble of disordered wires. Our results are representative for wires made of a normal metal as well as of a 2D electron gas at a semiconductor heterointerface.

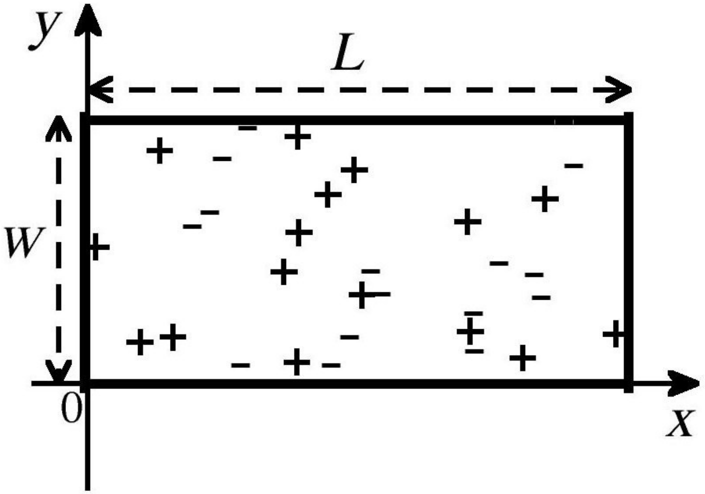
The single electron wave functions $\varphi(x, y)$ at the Fermi energy E_F in the wire obey the Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+V(x, y)+U_I(x, y)\right]\varphi(x, y)=E_F\varphi(x, y),$$

where $V(x , y)$ is the potential describing the wire edges and $U_I(x , y)$ is the potential due to the impurity disorder.

Models of disorder used in our calculations

Impurities



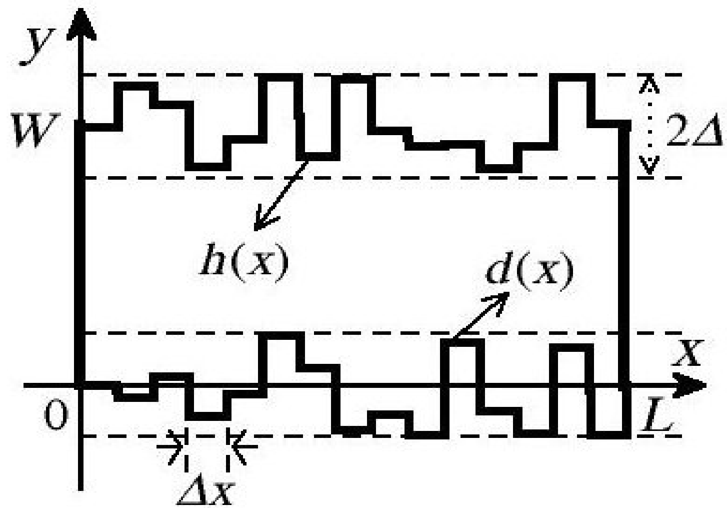
The sign of the impurity strength γ and impurity positions (x_i, y_i) are varied at random. The impurity potential is

$$U_I(x,y)=\sum_i \gamma\,\delta(x-x_i)\,\delta(y-y_i).$$

The wire has smooth edges

$$V(x,y)=\begin{cases}0, & for\ \ 0<y<W\\ \infty, & outside\ \ (0,W)\end{cases}.$$

Edge roughness



This wire is without impurities:

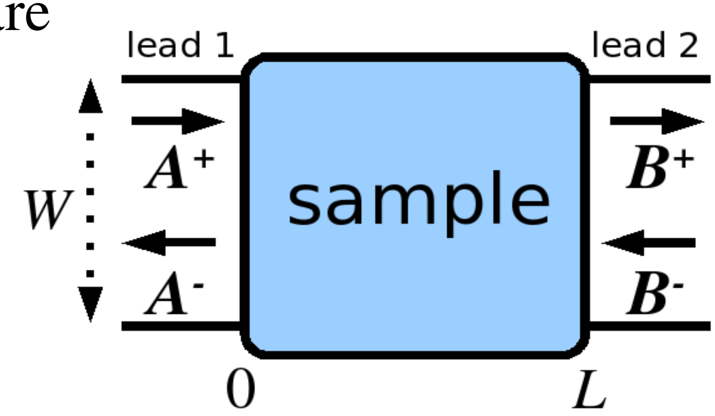
$$U_I(x,y)=0.$$

The wire edges, $h(x)$ and $d(x)$, are the step functions with the amplitude Δ and constant step length (correlation length) Δx. The edge potential is

$$V(x,y)=\begin{cases}0, & for\ \ d(x)<y<h(x)\\ \infty, & outside\ \ (d(x),h(x))\end{cases}.$$

Consider the wire connected to two perfect semi-infinite leads of width W.

The transverse wave functions (channels) in the leads are



$$\chi_n(y) = \begin{cases} \sqrt{2/L}\sin(\pi n y/W), \ for \ 0<y<W \\ 0, \ outside \ (0,W) \end{cases} .$$

The total wave function reads

$$\varphi(0,y) = \sum_{n=1}^{N} \left[A_n^+(0) + A_n^-(0)\right]\chi_n(y)$$

at $x = 0$ (in the lead 1) and

$$\varphi(L,y) = \sum_{n=1}^{N} \left[B_n^+(L) + B_n^-(L)\right]\chi_n(y)$$

at $x = L$ (in the lead 2). Here

$$A_n^+(x) = a_n^+ e^{ik_n x}, \ A_n^-(x) = a_n^- e^{-ik_n x},$$

and analogously for $B_n^+(x)$ and $B_n^-(x)$, where k_n is the wave vector in the channel n at energy

$$E_F = \epsilon_n + \frac{\hbar^2 k_n^2}{2m}$$

and $\epsilon_n = \hbar^2\pi^2 n^2/2mW^2$ is the eigenenergy of state $\chi_n(y)$.

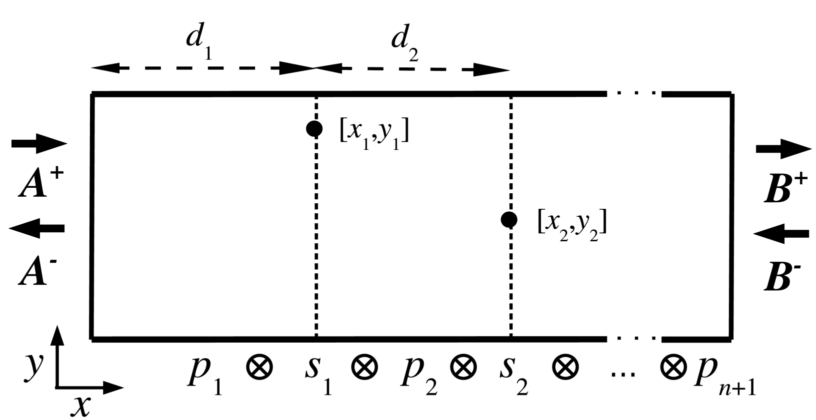
The scattering-matrix approach

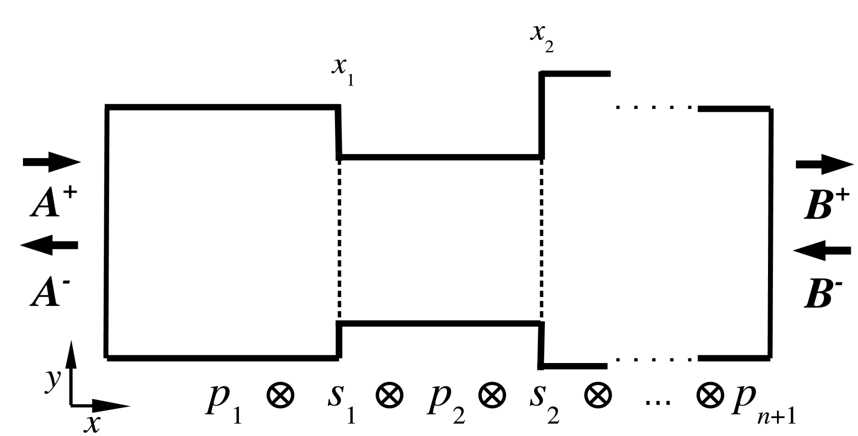
The incoming amplitudes $\boldsymbol{A}^{+}$ and $\boldsymbol{B}^{-}$ are related to the outcoming amplitudes $\boldsymbol{A}^{-}$ and $\boldsymbol{B}^{+}$ through the scattering matrix S as

$$\begin{pmatrix} A^{-} \\ B^{+} \end{pmatrix} = \begin{bmatrix} r & t' \\ t & r' \end{bmatrix} \begin{pmatrix} A^{+} \\ B^{-} \end{pmatrix},$$

where $\boldsymbol{A}^{\pm}$ and $\boldsymbol{B}^{\pm}$ are $N \times 1$ vectors and t, r, t', r' are the $N \times N$ matrices. In particular, $t_{n n'}$ is the transmission amplitude across disorder from the channel n to the channel n' and $r_{nn'}$ is corresponding reflection amplitude.

The S-matrix of the disordered sample can be expressed as a product of S-matrices of the individual scaterrers which constitute disorder [6-8].





The Landauer conductance

At zero temperature, the conductance (in units $2e^2/h$) of the disordered wire is given by the Landauer formula

$$g = \sum_{n=1}^{N_c} T_n = \sum_{n=1}^{N_c} \left(\sum_{n'=1}^{N_c} \frac{k_{n'}}{k_n} |t_{nn'}|^2 \right), \qquad (1)$$

where we sum over all N_C conductive channels. Here T_n are the transmission probabilities through disorder for the electron impinging disorder in the n-th conducting channel.

In the ensemble of macroscopically identical wires disorder fluctuates from wire to wire and so does the conductance. Hence it is meaningful to evaluate (1) for the ensemble of wires and to study the ensemble-averaged conductance $\langle g \rangle$, variance $[\, \langle g^2 \rangle - \langle g \rangle^2 \,]^{1/2}$, resistance $\langle 1/g \rangle$, ...

Analytical formulas for the wires with white-noise disorder (impurities)

The theory of Anderson localization (see e.g. [9]) predicts for the mesoscopic Q1D wire following transport regimes:

1) weak localization regime, where $l \ll L \ll \xi$ and $\xi = N_C l$ is the localization length

   The average conductance of the wire consists of the classical Ohmic term minus small weak localization correction

$$\langle g \rangle = \sigma_{dif} W/L - 1/3,$$

   where $\sigma_{dif} = \pi n_e l/k_F$ is the diffusive conductivity, k_F is the 2D Fermi wave vector and $n_e = k_F^2/2\pi$ is the 2D electron density. The average resistance linearly increases

$$\langle \rho \rangle = \langle 1/g \rangle = \rho_C + \rho_{dif} L/W,$$

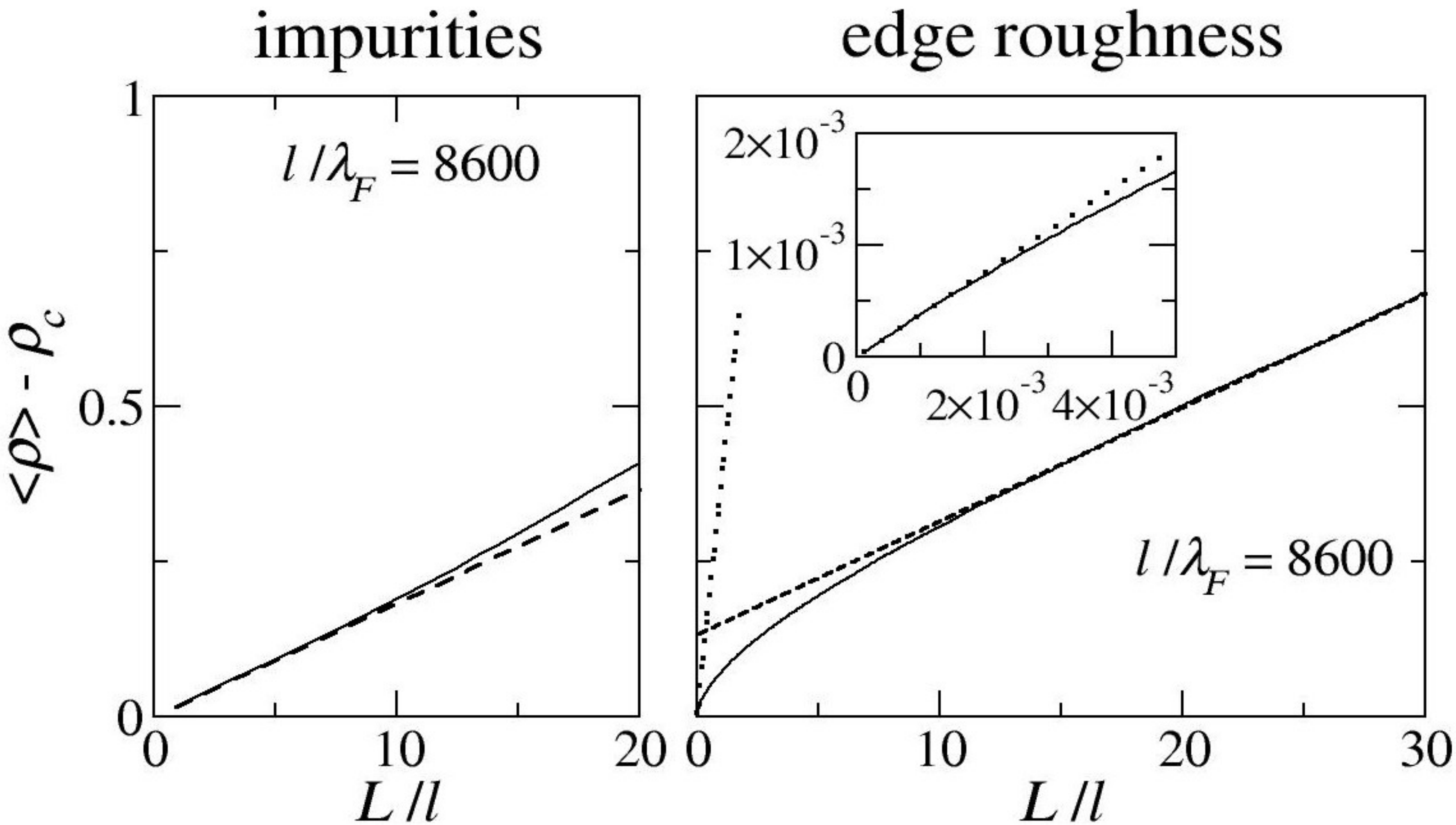
   where $\rho_C = 1/N_C$ is the contact resistance and $\rho_{dif} = 1/\sigma_{dif}$ is the diffusive resistivity. The conductance fluctuations are length-independent (universal)

$$\mathrm{var}(g) = \sqrt{\langle g^2 \rangle - \langle g \rangle^2} = 0.365.$$

2) strong localization regime, where $\xi \ll L$

   The conductance/resistance exponentially decreases/increases with L and typical conductance obeys the formula $\langle \ln g \rangle = -L/\xi.$

Numerical results for uncorrelated roughness ($\Delta x < \lambda_F$)



In the quasi-ballistic and diffusive regime the resistance obeys the standard linear increase

$\langle\rho\rangle = 1/N_C + \rho_{dif} L/W$ (dashed line)

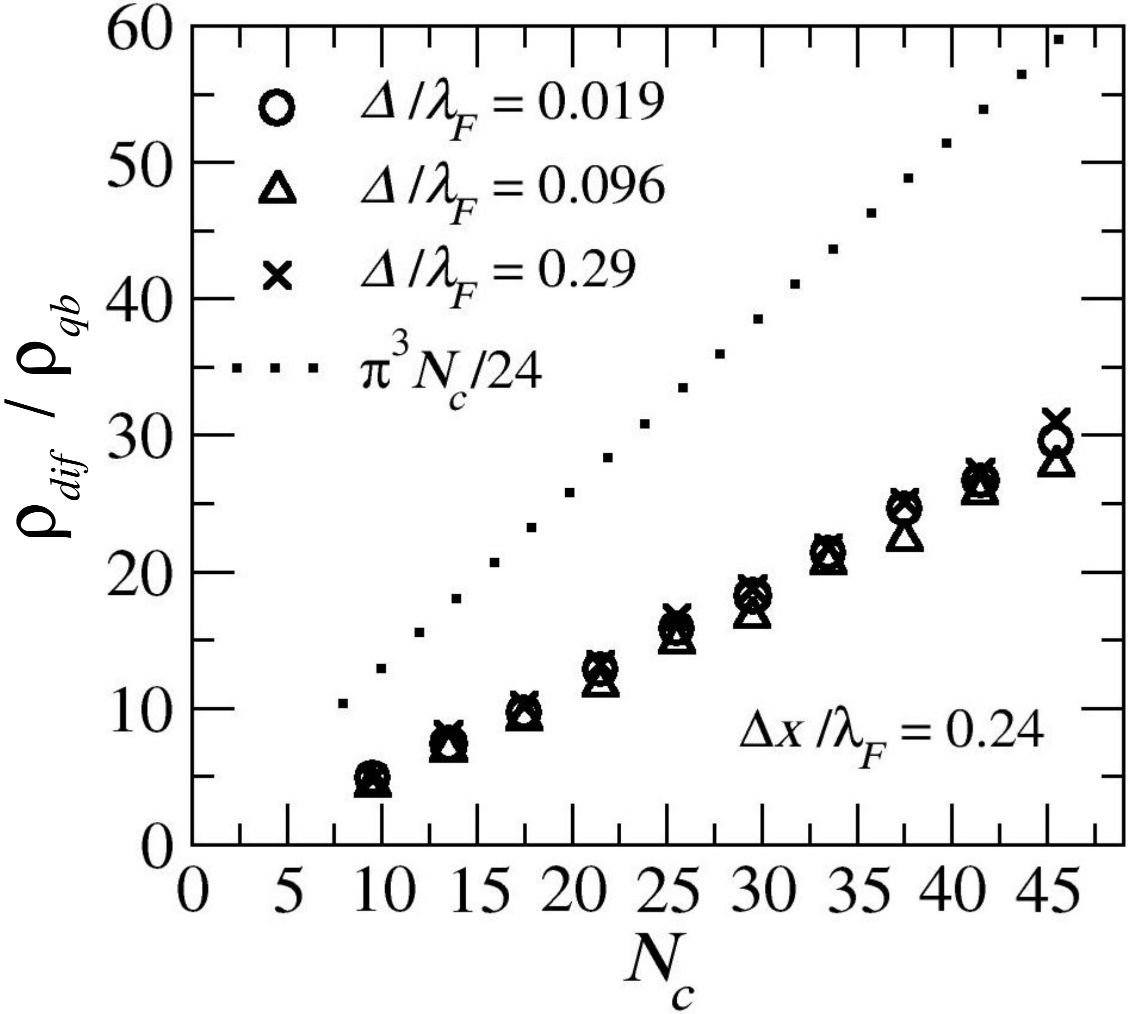
In the quasi-ballistic regime ($L \ll l$):

$\langle\rho\rangle = 1/N_C + \rho_{qb} L/W$, (dotted line)

In the diffusive regime ($l \ll L \ll \xi$):

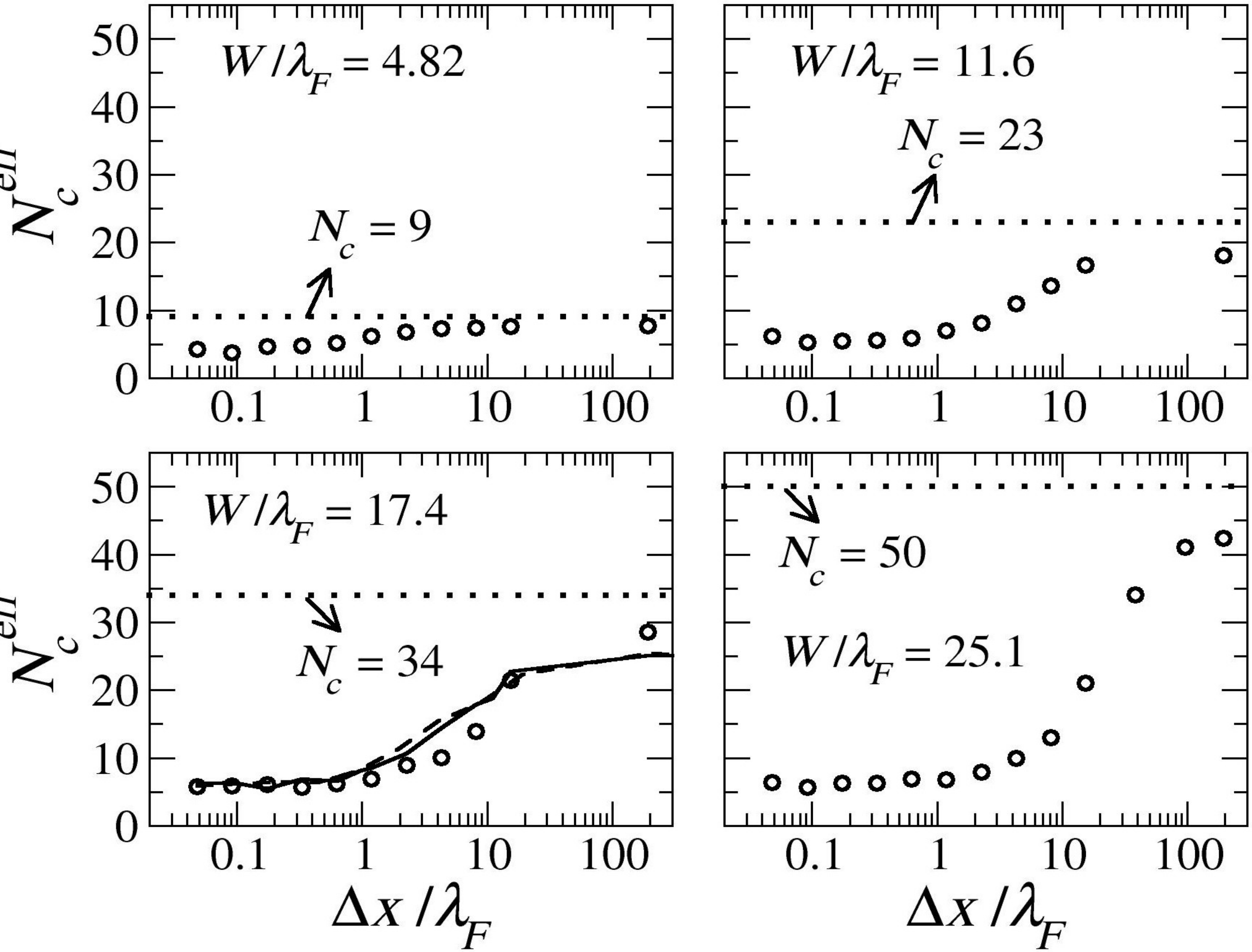
$\langle\rho\rangle = 1/N_C^{eff} + \rho_{dif} L/W$, (dashed line)

edge roughness ($\Delta x < \lambda_F$)

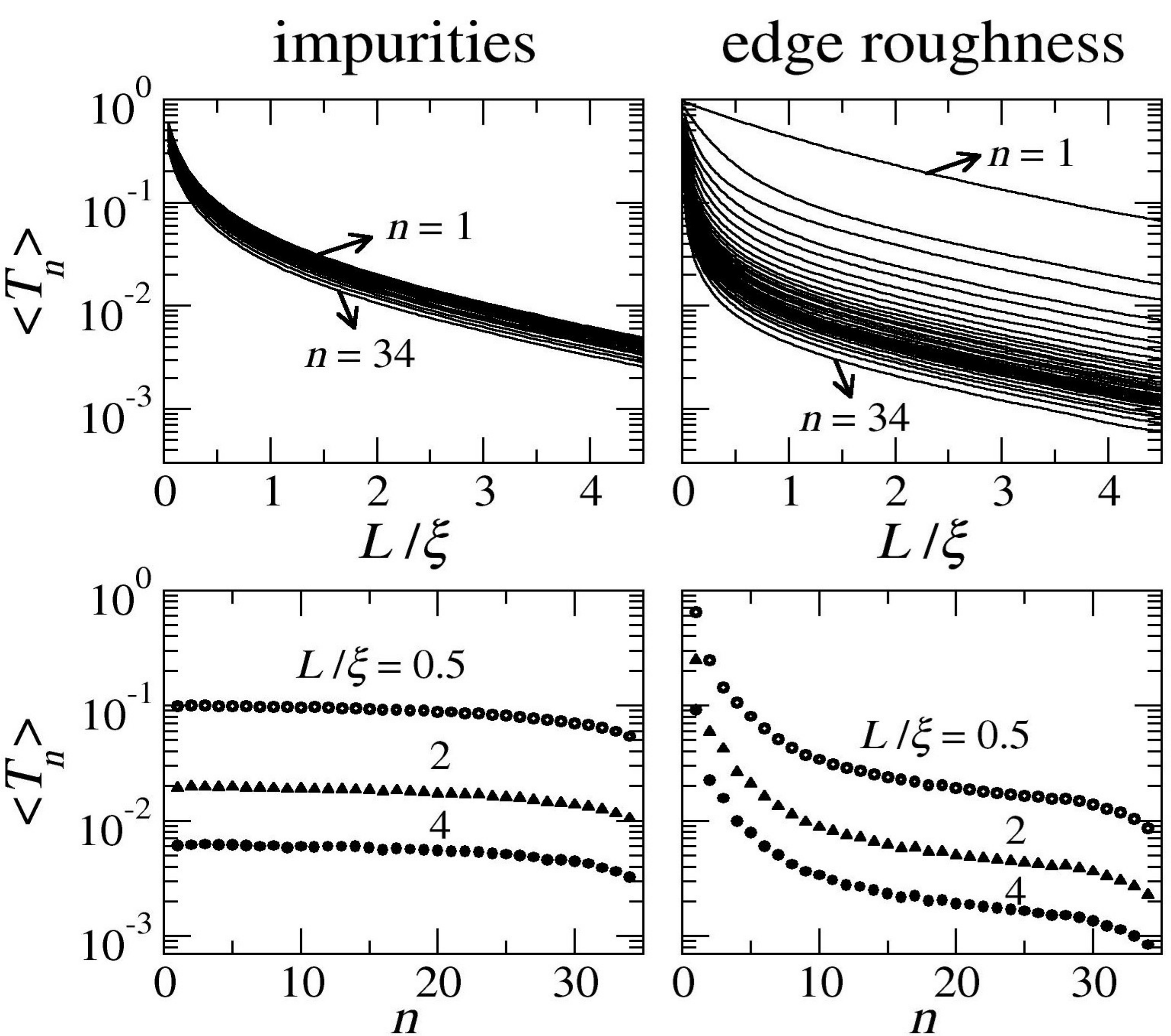


The ratio of the quasi-ballistic resistivity ρ_{qb} to the diffusive resistivity ρ_{dif} is ~ N_c independently on the parameters of roughness.

edge roughness



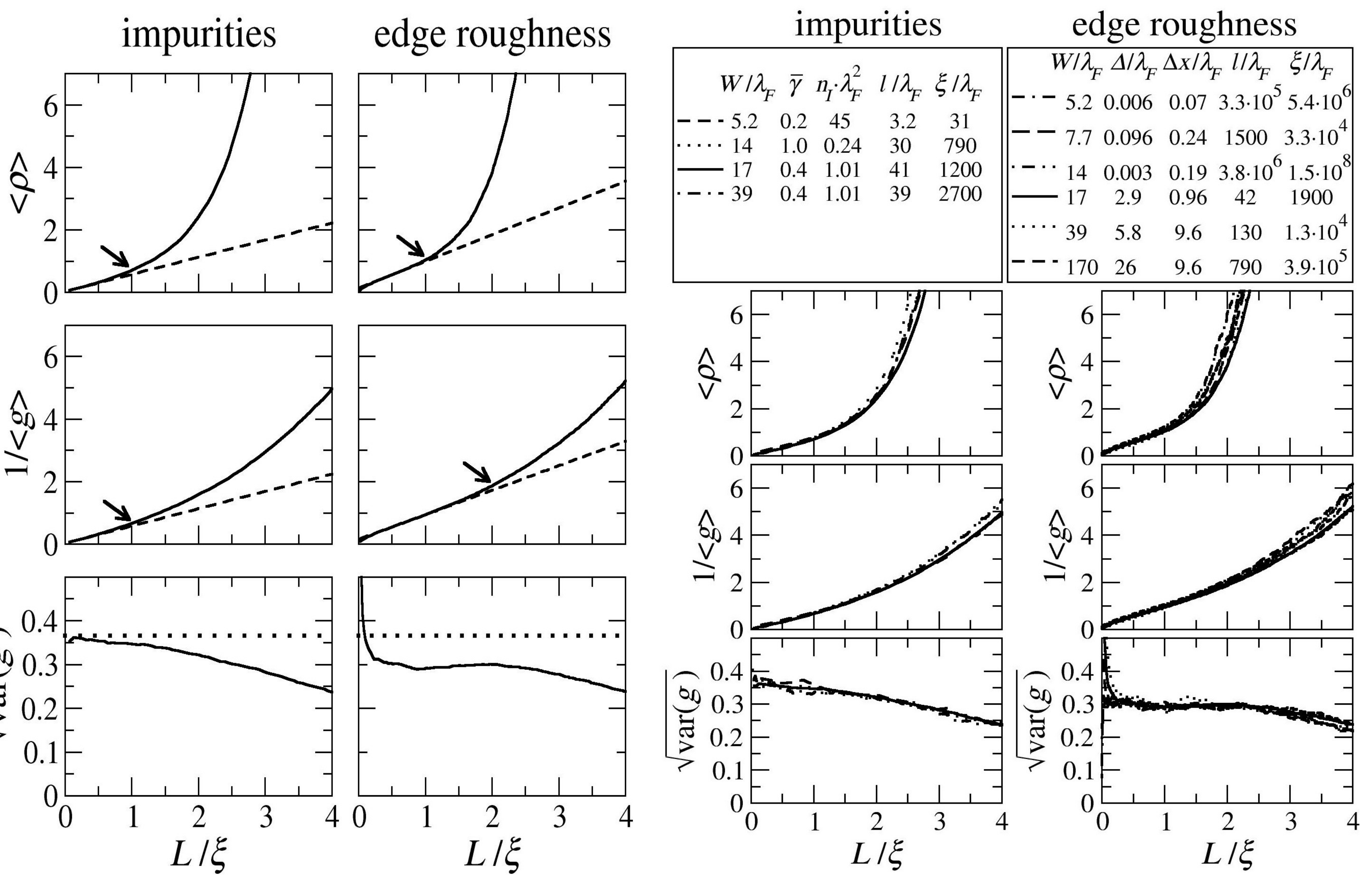
Transport in the diffusive regime is carried by a small effective number of open channels $N_C^{eff} \sim 6$. This number is universal - independent on N_c and on the parameters of roughness.



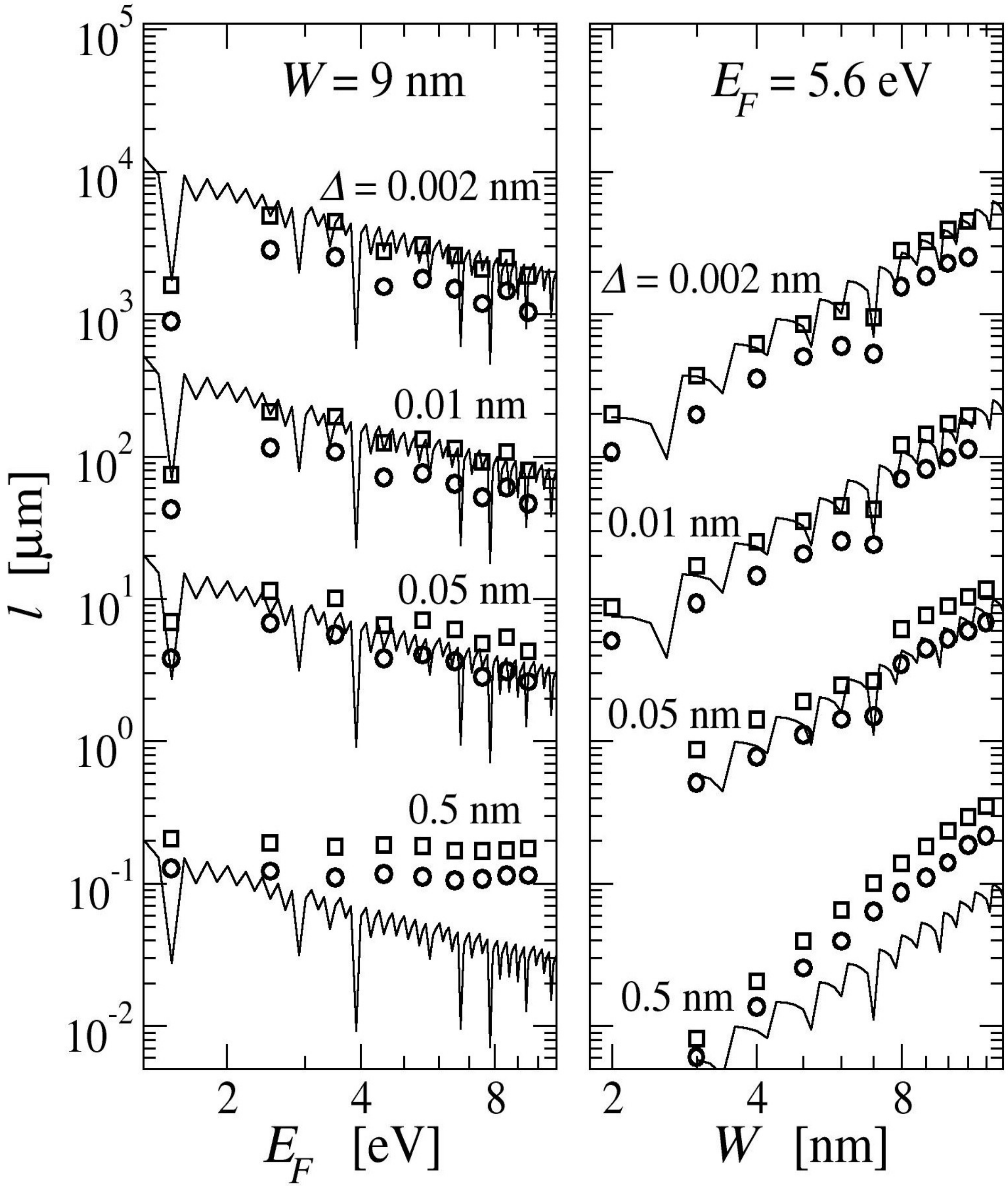
The average channel transmissions $\langle T_n \rangle$ are equivalent $\langle T_1 \rangle = \langle T_2 \rangle = ... = \langle T_{N_c} \rangle$ and in the diffusive regime

$$\langle T_n \rangle \sim l/L.$$

In the wire with edge roughness $\langle T_n \rangle$ decay fast with raising n because scattering by rough edges is weakest in the channel $n = 1$ and strongest in the channel $n = N_C$.



For edge roughness $1/\langle g\rangle$ rises linearly with the L (a sign of the diffusive regime) up to the $L \sim 2\xi$. Moreover we observe a tendency of a single parameter scaling.



solid line – semiclassical electron mean-free path l_{Boltz} derived from the Boltzmann equation

squares – numerically calculated semiclassical mean-free path l_{clas}

circles – numerically calculated quantum mean-free path l

In Au wire, l_{Boltz} agrees with l_{clas} only for the unrealistic small roughness amplitude Δ and both semiclassical mean free paths are at least about 2 times larger than quantum l.

Conclusions

We first study the impurity-free wire whose edges have roughness with a correlation length comparable with the Fermi wave length. Simulating wires with the number of the conducting channels (N_c) as large as 34 - 347, we observe the roughness-mediated effects which are not observable for small N_c (~ 3 - 9) used in previous works:

1) We observe the crossover from the quasi-ballistic transport to the diffusive one, where the ratio of the quasi-ballistic resistivity to the diffusive resistivity is ~ N_c independently on the parameters of roughness.

2) We find that transport in the diffusive regime is carried by a small effective number of open channels, equal to ~ 6. This number is universal - independent on N_c and on the parameters of roughness.

3) We see that the inverse mean conductance rises linearly with the wire length (a sign of the diffusive regime) up to the length twice larger than the electron localization length.

4) We develop a theory based on the weak-scattering limit and semiclassical Boltzmann equation, and we explain the first and second observations analytically. For impurity disorder we find a standard diffusive behavior.

5) We derive from the Boltzmann equation the semiclassical electron mean-free path and we compare it with the quantum mean-free path obtained from the Landauer conductance. They coincide for the impurity disorder, however, for the edge roughness they strongly differ, i.e., the diffusive transport in the wire with rough edges is not semiclassical. It becomes semiclassical only for roughness with large correlation length. The conductance then behaves like the conductance of the wire with impurities, also showing the conductance fluctuations of the same size.

References

[1] Y. Imry, *Introduction to Mesoscopic Physics* (Oxford University Press, Oxford, UK, 2002)

[2] S. Datta, *Electronic Transport in Mesoscopic Systems* (Cambridge University Press, Cambridge, UK, 1995).

[3] P. A. Mello and N. Kumar, *Quantum Transport in Mesoscopic Systems* (Oxford University Press, Oxford, UK, 2004).

[4] L. Saminadayar, C. Bauerle, and D. Mailly, in *Encyclopedia of Nanoscience and Nanotechnology*, edited by H. S. Nalwa (American Scientific, Valencia, CA, 2004), Vol. **3**, pp. 267-285.

[5] J. Feilhauer and M. Mosko, arXiv:1011.6193v2 [cond-mat.mes-hall] (accepted to Phys. Rev. B)

[6] H. Tamura and T. Ando, Phys. Rev. B **44**, 1792 (1991)

[7] M. Cahay et al., Phys. Rev. B **37**, 10125 (1988)

[8] J. A. Torres and J.-J. Saenz, J. Phys. Soc. Jpn. **73**, 2182 (2004)

[9] P. Markoš, Acta Physica Slovaca **56**, 561 (2006)

Acknowledgements

We thank for the grant VVCE-0058-07, VEGA grant 2/0633/09, and grant APVV-51-003505.