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Electron transport through quantum wires and point contacts

Published in:
PHYSICAL REVIEW B

DOI:
10.1103/PhysRevB.70.233308

Published: 17/12/2004

Please cite the original version:
We have studied quantum wires using the Green’s function technique within density-functional theory, calculating electronic structures and conductances for different wire lengths, temperatures, and bias voltages. For short wires, i.e., quantum point contacts, the zero-bias conductance shows as a function of the gate voltage and at a finite temperature a plateau at around $0.7G_0$. ($G_0=2e^2/h$ is the quantum conductance.) The behavior, which is caused in our mean-field model by spontaneous spin polarization in the constriction, is reminiscent of the so-called 0.7 anomaly observed in experiments. In our model the temperature and the wire length affect the conductance–gate-voltage curves similarly as in experiments.

DOI: 10.1103/PhysRevB.70.233308  PACS number(s): 73.63.Nm, 73.21.Hb

In this work we use DFT to investigate the spontaneous spin polarization and its consequences for the conduction in QW’s. In contrast to the model Hamiltonian studies we can take the actual geometry and the effects of the gate potential directly into account. The use of the Green’s function technique allows us to study real open systems with infinite electrodes even in the nonequilibrium case under a finite bias voltage. However, we keep the model geometry simple in order to obtain physically transparent results and we study to what extent the mean-field DFT model can describe the experimental findings. The previous papers have typically concentrated on one QPC or QW structure whereas we study systematically the influence of the QW geometry, the temperature, and the bias voltage.

Below we use in the equations effective atomic units which are derived by setting $\epsilon = h = m_e = m^* = e = 1$. $m^*$ and $\epsilon$ are the relative effective electron mass and the relative dielectric constant, respectively. For GaAs $m^* = 0.067$ and $\epsilon = 12.7$ and the effective atomic units of length and energy are $\alpha_0 = 10.0307$ nm and $H_0^* = 11.3079$ meV, respectively. We use these relations to convert the model parameters and results to values comparable with real systems.

Our quasi-2D model for a QW is shown in Fig. 1. The calculation area $\Omega$ consists of the QW and parts of the electrodes. The gray areas denote the rigid positive background charge of the electrodes. The electrodes continue to infinity outside the calculation region. The uniform background charge density is varied in the black wire region in order to model the effects of the gate voltage.

FIG. 1. 2D quantum wire between two electrodes. The gray areas denote the rigid positive background charge of the electrodes. The electrodes continue to infinity outside the calculation region. The uniform background charge density is varied in the black wire region in order to model the effects of the gate voltage.
todes. The semi-infinite electrodes include the positive background charge with the constant density of $0.2 a_0^{-2}$ $\approx 2 \times 10^{11} e/cm^2$, which is a typical experimental value for the 2D electron gas at the interface, and the neutralizing 2D electron gas with the density $\rho(r)$. The electron density deep in the electrodes in the regions $\Omega_{LR}$ is assumed to coincide with that in an infinite uniform wire. The QW between the electrodes is also modeled using a rigid uniform positive background charge (the black region in Fig. 1). We vary this positive charge density in order to mimic the effects of a gate voltage, i.e., we define the gate voltage as the Coulomb potential due to this charge at the midpoint of the QW. At both sides of the electrodes and the wire we include enough empty vacuum, and the electron density is required to vanish at the boundaries $\partial \Omega_{L/R}$.

We employ the DFT within the local density approximation (LDA) for the electron exchange and correlation and calculate the electron density using Green’s functions as

$$\rho(r) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \text{Im}[G^\ast(r, r'; \omega)] d\omega. \tag{1}$$

Above, $G^\ast(r, r'; \omega)$ is the so-called lesser Green’s function and the integration is over all energy values. $G^\ast(r, r'; \omega)$ has to be solved self-consistently with respect to the electron density and the effective potential and using open boundary conditions at $\partial \Omega_{LR}$ (see, e.g., Ref. 12). The effective potential consists of the usual Coulomb potentials due to the positive and negative charge densities and the exchange-correlation potential within the LDA. It may also include a ramp potential which takes into account a possible bias voltage between the electrodes. The scheme is computationally much more demanding than solving for the wave functions of a finite system. However, it has the important advantages that finite-size effects are vanishingly small due to the open boundary conditions and that the effects of a finite bias are calculated self-consistently in nonequilibrium.

For a finite bias the electric current is calculated as

$$I = \frac{1}{\pi} \int_{-\infty}^{\infty} T(\omega)[f_L(\omega) - f_R(\omega)] d\omega, \tag{2}$$

where the Fermi functions $f_L$ and $f_R$ are shifted with respect to each other by the bias voltage $V_{sd}$. $T(\omega)$ is the tunneling probability and it is calculated using the Green’s functions. In the zero-bias limit $f_L(\omega) = f_R(\omega) = f(\omega)$ and one obtains the linear-response conductance as

$$G = \frac{1}{\pi} \int_{-\infty}^{\infty} T(\omega) \frac{df(\omega)}{d\omega} d\omega. \tag{3}$$

At zero temperature the conductance is simply $T(\omega_f)$, where $\omega_f$ is the Fermi energy. At a finite temperature also electron states with energies near the Fermi level contribute to the conductance, as the derivative of the Fermi function $f(\omega)$ differs from the $\delta$ function. A finite temperature influences the solution also through the electron density. Below we show also differential conductances corresponding to given bias voltages at zero temperature. We determine them by increasing the bias voltage slightly and calculating the derivative $dl/dV_{sd}$ numerically.

We have implemented the nonequilibrium DFT scheme using the finite-element method as explained in our paper.\textsuperscript{13} We use 2D high-order polynomial bases\textsuperscript{14} up to the fourth order in order to reduce the basis size. In a typical calculation the number of basis functions needed to reach sufficient accuracy is $\approx 2800$ for high-order polynomials compared to $\approx 5500$ for low-order polynomials.

We have studied the electron structures of several QW’s of different lengths $[L = (5-10) a_0^\ast]$ and widths $[S = (5-10) a_0^\ast]$ and determined their conductance as a function of the gate voltage. The width of the electrodes $W = 20 a_0^\ast$ used is clearly larger than those of the QW’s. The widest QW’s show the typical conductance staircase as a function of the gate voltage. For the narrowest QW’s our model predicts prominent electron resonance states. They are evident as peaks in the local density of states (LDOS) (see Fig. 5 below). They can be thought to result as interference of the waves transmitted and reflected at the ends of the QW but, on the other hand, the resonances contain also characteristics of the DOS in quasi-one-dimensional wires. The resonance peaks are broader in short and wide QW’s than in long and thin QW’s, because short QW’s are more strongly connected to the electrodes. If the resonance peaks are narrow enough, a spontaneous spin polarization occurs in a limited range of gate voltages. One solution with spin polarization in the QW is shown in Fig. 2 which gives the total electron density and the difference between the spin-up and spin-down densities.\textsuperscript{6} Berggren and Yakimenko,\textsuperscript{8} and Starikov et al. have also found spin-polarized solutions in their DFT calculations for QPC’s. They used models which correspond most closely to the shortest QW’s of our calculations. The broad resonances found by Meir et al. and the nonappearance of the resonances in the calculation by Starikov et al. are therefore in agreement with the trend of our results.

Below we are concerned mainly with the conductance plateaus below $1 G_0$ and therefore we discuss only narrow
gates are used. They control not only the potential level in
and theory may be due to the fact that in experiments side
the wire increases. The differences between the experiment
G
lower and forms a clear peak below 0.5

G
are shown in Fig. 3 as a function of the gate voltage and at
zero temperature. The figure shows clearly the effect of the
temperature happens. The conductances of wires of different lengths
appearing. The length dependence of the conductance among
the widths of the resonance peaks. Therefore \(G_0\) decreases. These findings are reminiscent of
the experimental temperature dependences.1,5

The reason for the different temperature behaviors of the
QW’s in our model can be seen in Fig. 5 which shows the
decomposition of the conductance of wire B into the spin-up
and spin-down electron contributions at two different
temperatures. As the temperature increases from 0 to 2 K spin
polarization increases at the gate voltages around the middle
of the plateau below \(1G_0\). At the same time, the (resonance)
peaks become also wider because more states contribute to
the conductance [see Eq. (3)]. The same behavior is seen also
for wires A and C. The reason for the increase in the
polarization is seen in the LDOS for wire B in the lowest part of
Fig. 5. When the temperature rises the electron density in-
creases in the QW due to the resonances near the Fermi
level. Then the decrease in the exchange-correlation energy
opens the spin gap, as can be seen in Fig. 5, and the polar-
ization increases. The effect is clearer for wire B than for
wires A and C. In wire A the electron density does not in-
crease as fast as in wire B because the resonance peaks are
wider. Wire C has a strong polarization already at zero tem-
perature and therefore it cannot show an increase as large as
wire B.

Our analysis of the temperature behavior is to a certain
extent parallel to the phenomenological model of Reilly et al.7
In their model the relevant parameter is the ratio between
the width of the spin gap and the thermal energy \(k_BT\) de-
termining the occupancy of the discrete spin-up and spin-down
energy levels. According to our calculations the temperature
broadening in the Fermi functions is small when compared to
the widths of the resonance peaks. Therefore \(k_BT\) has to be

1,5

FIG. 3. Conductance as a function of the gate voltage for QW’s
with width \(S=5a_0\) and with different lengths \(L\). The width of the
electrodes is \(W=20a_0\), and the length of the computational area is
\(A=47a_0\) (see also Fig. 1). The successive curves have been shifted
by 0.5\(G_0\). The conductance of the wire with \(L=10a_0\) is decomposed
into spin-up and spin-down contributions (dotted lines).

wires with width \(S=5a_0\), where spontaneous spin polarization
happens. The conductances of wires of different lengths
\(L\) are shown in Fig. 3 as a function of the gate voltage and at
zero temperature. The figure shows clearly the effect of the
electrode-wire connection. The long wires have clear peaks
due to resonances. The heights of the peaks are 0.5\(G_0\), meaning
that only a single electron polarized mode contributes to
them. The wires with lengths \(L=(6–8)a_0\) exhibit resonances
which are just narrow enough for the spin polarization to
appear. The length dependence of the conductance among
these three wires is in qualitative agreement with the recent
measurements for QW’s by Reilly et al.3 That is, although
the wires in the experiments are clearly longer than in our
calculations, the structure around \((0.5–0.7)G_0\) becomes
lower and forms a clear peak below 0.5\(G_0\) when the length of
the wire increases. The differences between the experiment
and theory may be due to the fact that in experiments side
gates are used.2 They control not only the potential level in
the QW, but also the width of the QW.

The effect of the temperature on the conductance behavior
of three QPC-like wires is shown in Fig. 4. At zero tempera-
ture, wire A \((L=6a_0)\) shows no plateau, whereas wire B \((L=
7a_0)\) has a plateau at \(\sim 0.7G_0\) and wire C \((L=8a_0)\) at
FIG. 4. Conductance as a function of the gate voltage for QW’s
with the width \(S=5a_0\) and lengths \(L=6a_0\) (wire A), \(7a_0\) (wire B)
and \(8a_0\) (wire C) at the temperatures of 0 K (solid curve), 2 K
(dashed curve), and 4 K (dotted curve).

\(\sim 0.5G_0\). When the temperature increases the plateaus below
\(1G_0\) in wires B and C shift downward and become smoother.
Wire A shows a weak temperature dependence so that the
slope at \(\sim 0.7G_0\) decreases. These findings are reminiscent of
the experimental temperature dependences.1,5

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termining the occupancy of the discrete spin-up and spin-down
energy levels. According to our calculations the temperature
broadening in the Fermi functions is small when compared to
the widths of the resonance peaks. Therefore \(k_BT\) has to be
replaced by the resonance peak width as the relevant parameter. Then the model can be used to explain the conductance–gate-voltage curves also at zero temperature.

The differential conductance of wire B at different bias voltages is shown in Fig. 6 as a function of the gate voltage. The increase in the applied bias voltage mainly increases the conductance but at the same time it also curtails the conductance plateaus. This is not exactly in agreement with the measurements, which show that the conductance plateau below \(1G_0\) rises with increasing bias voltage.\(^4,5\) According to our calculations the rise of \(V_{sd}\) diminishes also the spin polarization in the QW. Our model cannot give the zero-bias anomaly behavior seen in experiments and explained as a Kondo phenomenon.\(^5,6\)

In conclusion, we have used density-functional theory and the Green’s function method to model the electronic structures and conductances of quantum wires. The dependence of the conductance on the length of the wire as well as on the temperature and the bias voltage dependences are reminiscent of experimental findings. However, our mean-field approach cannot reproduce the zero-bias anomaly.

We acknowledge generous computer resources from the Center for Scientific Computing, Espoo, Finland. This research has been supported by the Academy of Finland through its Centers of Excellence Program (2000-2005). P.H. acknowledges financial support by the Vilho, Yrjö, and Kalle Väisälä Foundation. We have used the Harwell Subroutine Library in our calculations.