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Quantum transport in cylindrical semiconductor nanowires with constrictions

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Abstract

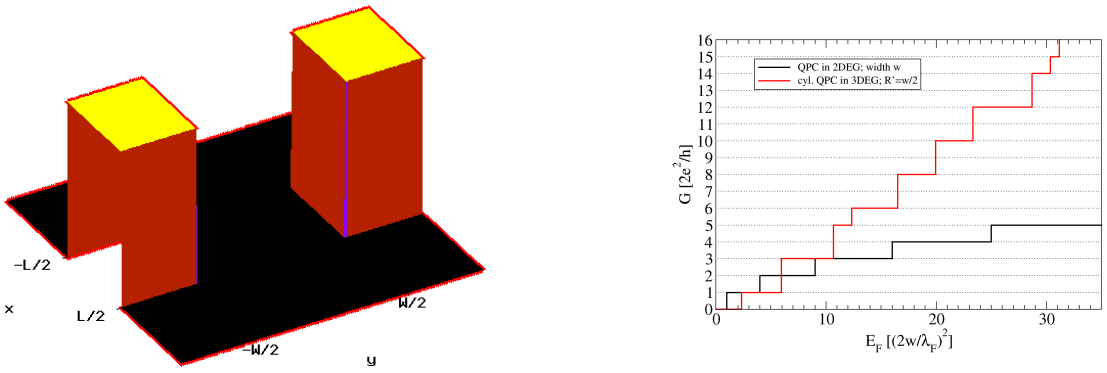
The energy dependence of the tunneling coefficient for a cylindrical semiconductor nanowire, i.e. a one-dimensional electron gas, with one or two constrictions is studied. Using the R-matrix formalism the localization probabilities at the resonant energies can be computed. They give decisive information about the physical meaning of the resonant peaks and dips that appear. The nanowire with two constrictions yields a well-defined system for the experimental evidence of the quasi-bound states of the evanescent channels. Clearly marked dips due to them should appear in the linear conductance at low temperatures.

1 Introduction

The quantum point contact (QPC) in a two-dimensional electron gas (2DEG) is nowadays, after 25 years, a well-known mesoscopic system that shows a striking quantum effect, namely the linear conductance at low temperatures is quantized in units of $2e^2/h$ in absence of magnetic field [1, 2]. This system is a clear experimental evidence of a ballistic conductor, whose electrical conductance is described by the two-terminal Landauer formula [3, 4, 5, 6, 7]. The measured quantized conductance is interpreted as the contact conductance for two-terminal systems multiplied with the total tunneling coefficient at the Fermi energy E_F

$$G(V_G) = \frac{2e^2}{h} Tr\{\boldsymbol{t}\boldsymbol{t}^\dagger\}(E_F; V_G), \tag{1}$$

where 2 is the spin degeneracy. The contact conductance e^2/h is due to the contact between a ballistic conductor, where elastic processes take place, and the two reservoirs, where dissipative processes take place [4, 9]. The $N \times N$ transmission matrix $\boldsymbol{t}$ describes the elastic scattering at the boundaries of the constriction, where N is the number of the conducting channels (i.e. open energy channels) in the leads. For a separable potential with no channel mixing [8], i.e. $t_{ij} = \delta_{ij}$, the trace yields an integer number, interpreted as the number of the conducting channels in the quantum point contact. The conductance steps are experimentally not perfectly sharp. Their shape can be explained in detail by the mode-conversion behavior at the interfaces between the narrow constriction and the wide 2DEG regions [5, 8]. The quantization in $G(V_G)$ appears because the boundaries of the constriction, especially its width w, change continuously with the gate voltage V_G, while the number of the conducting channels at the Fermi energy changes necessarily stepwise, see Fig. 1. The above formula gives also an explanation for the resonant structure of the conductance steps in case of sufficiently long constrictions [5, 10]. The conductance of the quantum point contact is proportional to the constriction width w but independent



(a) (b)

Figure 1: (a) A simple rectangular confinement potential in the plane of a 2DEG for modeling a constriction of width w and length L; x is the transport direction, while y is the confinement direction. (b) Idealized quantized conductance at low temperatures for a constriction of the same width $w = 2R'$ in 2DEG and in 3DEG.

of its length L, as long as it is long enough such that the evanescent channels do not play an important role [5]. Furthermore, Eq. (1) helps to understand the experimental washing out of the steps in case of an energy averaging, either due to a finite temperature [11] or due to a finite source-drain bias [12].

The quantization of the conductance is not restricted to constrictions in 2DEG. It also appears for constrictions in a three-dimensional electron gas (3DEG). Many theoretical [13, 14, 15, 16, 17, 18, 19, 20, 21, 22] and experimental [23, 24] studies analyze the quantization of the conductance of metallic particles or quantum wires between two 3DEGs. One difference to the case of 2DEG is that the sequence of the conductance steps is given by the degeneracy of the transversal modes that depends on the geometry of the cross-section of the constriction [24, 15]. For example, for a cylindrical constriction the linear conductance increases either in steps of $2e^2/h$ or $4e^2/h$ (i.e. two quantum conductance units), because of the azimuthal degeneration: the quantum numbers m and $-m$ contribute equally to the conductance [14], see Fig. 1(b). In Fig. 1(b) the quantized conductance for a cylindrical constriction in a 3DEG is compared to the quantized conductance for a constriction with the same width $w = 2R'$ in a 2DEG. As one can see, at the same Fermi energy (i.e. at the same gate voltage V_G), there are much more conducting channels open in the case of a cylindrical quantum point contact. All the studies in 3DEG treat only one constriction and they were driven by the idea to determine the cross section of an atomic-scale contact or of a small connecting metallic nanowire from the conductance measurements.

In the last few years the interest in the semiconductor nanowires has increased progressively. Semiconductor nanowires are structures with an extremely high aspect ratio and a diameter less than 100 nm. Nowadays, almost all semiconductor materials can be grown as nanowires. The carrier confinement in two directions make them very attractive for applications in nano-opto-electronic devices [25, 26]. One could produce constrictions

also in nanowires by different methods. One method could be to define the constrictions electrostatically, like in the first experiments [1, 2] so that the width, i.e. the radius, of the constrictions can be changed by an external gate voltage [27]. But for the nanowires, it is possible to define a quantum point contact by incorporating a double-barrier potential [28], even though the variation of the width of the constriction is not so easy. The constrictions can be also produced by etching the nanowires or growing nanowire heterostructures with different diameters. In those cases where the width of the constrictions are fixed the conductance measurements are done by varying the Fermi energy by illuminating the sample [2, 29]. A nanowire with a constriction provides a simple well-defined structure for studying both theoretically and experimentally the quantum point contact in a one-dimensional electron gas.

In this paper we study the tunneling coefficient in a cylindrical semiconductor nanowire with one or two symmetric rectangular constrictions. Doping the ends of the nanowire, the Fermi wavelength becomes comparable to the width of the nanowire and the mean free path between the contacts may be larger than the nanowire length. Thus, the nanowire becomes an ideal system for studying the ballistic transport of electrons. A proper modeling of the ballistic transport in semiconductor nanowires can be performed only in the frame of quantum mechanics, either microscopic modeling (i.e. first principles or ab-initio) or mesoscopic modeling (i.e. within effective mass approximation). The tunneling coefficient is the key quantity for the linear conductance in mesoscopic systems, see Eq. (1). We use the R-matrix formalism [30, 31, 32, 33, 34, 35] for solving the multi-channel scattering problem in cylindrically symmetric systems. So that, this method allows the computation of the tunneling coefficient very efficiently. Furthermore, this method allows the computation of the scattering wave functions inside the scattering region. The mapping of the localization probabilities inside the scattering region helps in the physical interpretation of the tunneling peaks and dips. A large energy interval is considered, so that we are beyond the single subband regime [36]. In Refs. [37, 38] cylindrical nanowires with two constrictions are analyzed but only between the first two thresholds and for the magnetic quantum number zero, i.e. $E \in [E^{(0)}_{\perp,1}, E^{(0)}_{\perp,2}]$. A resonant tunneling effect is evidenced and it is shown that the width of the resonant peaks decreases with decreasing the cross-section of the constrictions. In this paper are presented results for higher energies and it is shown that the region between the two constrictions plays the role of an attractive potential. It was shown that an attractive scattering potential either in a quantum wire [39, 40, 41, 36, 42, 43] or in a nanowire [34] yields quasi-bound states of evanescent channels that appear as dips in the transmission coefficient. Also quantum point contacts with impurities were subjects of theoretical [44, 45, 46, 47] as well as experimental studies [48, 49, 50, 51, 52]. The experimental realizations of quantum point contacts with impurities, especially with attractive impurities, introduce unwanted effects, such that the interpretation of the measured conductance is not straightforward. The nanowire with two constrictions is a much simpler structure that could offer an ideal system for studying the quasi-bound states of the evanescent channels. The effective attractive potential is provided by the nanowire itself.

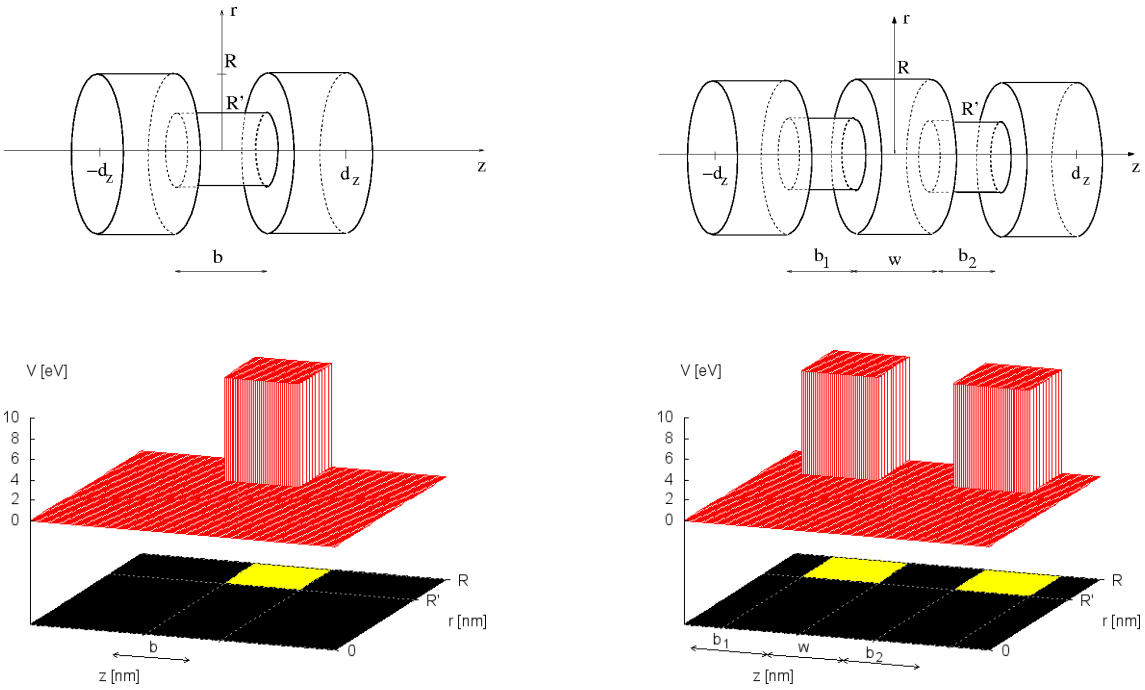


Figure 2: Sketches of a nanowire with one or two constrictions and the corresponding scattering potential $V(z,r)$ in the reduced two-dimensional model.

2 Model

We consider in this paper a cylindrical semiconductor nanowire with one or two rectangular constrictions of width b and separation w, see Fig. 2. The constrictions can be produced by different techniques as is discussed in the introduction. We are aware that rectangular constrictions are an idealization, but they offer the most pronounced resonant features [5, 53].

We model the electronic transport in semiconductor nanowires within the single-band effective mass approximation. Details of our method for cylindrically symmetric systems are given in Ref. [34]. We introduce here very shortly some terms and definitions. The envelope functions are computed as solutions of the Schrödinger type equation

$$\left[-\frac{\hbar^2}{2}\nabla\cdot\left(\boldsymbol{M}(\boldsymbol{r})^{-1}\nabla\right)+V(\mathbf{r})\right]\Psi(\mathbf{r})=E\Psi(\mathbf{r}), \tag{2}$$

with scattering boundary conditions [34]. For a layered heterostructures one has to use a position dependent effective mass tensor $\boldsymbol{M}(\mathbf{r})^{-1}$, but in the case of nanowires with constrictions one can consider a position-independent mass tensor $\boldsymbol{M}$. Depending on the material and on the crystal growth orientation, one can have an isotropical effective mass tensor, which is the case we consider in this paper. The extension of the model for position-dependent and anisotropic effective mass tensor is also possible [54].

The scattering potential $V(\mathbf{r})$ has a position dependence only inside the scattering region $z\in[-d_z,d_z]$ and is constant or separable in the asymptotic regions, i.e. leads $|z|>d_z$.

We consider here the case of constant potentials in the leads, i.e. $V(r, z < -d_z) = V_1$ in the source and $V(r, z > d_z) = V_2$ in the drain and hard-wall confinement inside the nanowire. In the linear regime we have the same potential in the leads, i.e. $V_1 \simeq V_2$. The scattering region has to include the constrictions, see Fig. 2.

Considering a cylindrical nanowire and a cylindrically symmetric scattering potential, one can reduce the tree dimensional scattering problem (2) to a series of two-dimensional scattering problems

$$\left[-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}-\frac{m^2}{r^2}+\frac{\partial^2}{\partial z^2}\right)+V(r,z)\right]\psi(E;r,z)=E\psi(E;r,z), \quad (3)$$

defined over an unbounded domain, i.e. $r \in [0, R], z \in (-\infty, \infty)$, where $m = 0, \pm 1, \pm 2, \ldots$ is the magnetic quantum number and describes the θ-dependence of the scattering wave function $\Psi(\mathbf{r}) = \psi(E; r, z)e^{im\theta}/\sqrt{2\pi}$. Each equation (3) for a specified m can be solved independently on other m values. In the asymptotic regions Eq. (3) is separable, so that the solutions are in these regions combinations of the transversal modes $\phi_n^{(m)}(r)$ multiplied by the incoming and outgoing plane waves along the z-direction $\exp(\pm ik_z z)$. Among all possible combinations, one chooses as suitable solutions the scattering states $\psi_{nm}^{(s)}(E; r, z)$, where the lead index s and the energy channel index n set up the incoming part of them. The coefficients of the outgoing combinations are the so-called multi-channel scattering matrix elements. The same coefficients give also the tunneling probabilities $T_{nn'}^{(m)}(E)$ for an electron incident in the lead s on energy channel n to be transmitted into the lead $s' \neq s$ on energy channel n'. A numerically efficient method to compute the multi-channel scattering matrix S is the R-matrix formalism [30, 31, 32, 33, 34, 35]. In general, one can not neglect in the above computation the contributions of the evanescent channels. The R-matrix formalism provides also the scattering wave functions inside the scattering region, whose localization probabilities give decisive information about the physical meaning of the resonant states.

The transversal modes $\phi_n^{(m)}(r)$ and their corresponding energies $E_{\perp,n}^{(m)}$ are solutions of the radial equation in the leads,

$$-\frac{\hbar^2}{2m^*}\left[\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}-\frac{m^2}{r^2}\right]\phi(r)=E_\perp\phi(r), \quad (4)$$

with Dirichlet (hard-wall) boundary condition on the surface of the cylindrical nanowire, i.e. $\phi_n(R) = 0$. The transversal modes are expressed in terms of the Bessel functions of the first kind, J_m and one has

$$E_{\perp,n}^{(m)}=\frac{\hbar^2}{2m^*}\left(\frac{x_{mn}}{R}\right)^2 \quad (5)$$

with x_{mn} the nth root of $J_m(x)$. These modes define the energy channels. All channels below the energy of the incident electron, i.e. $E_{\perp,n}^{(m)} < E$, are called conducting or open channels. For a given energy E there is finite number of open channels in each asymptotic region, i.e. $s = 1, 2$ for source and drain, respectively, and all other channels are called evanescent or closed channels.

Following the Landauer formula [3, 4, 7] the linear conductance for a cylindrical nanowire with a scattering potential $V(z,r)$ at zero temperature is defined as

$$G = \frac{2e^2}{h}\sum_m T^{(m)}(E) = \frac{2e^2}{h}\sum_m\sum_{n,n'} T^{(m)}_{nn'}(E), \tag{6}$$

where $T^{(m)}(E) = \sum_{n,n'} T^{(m)}_{nn'}(E)$ is the total tunneling coefficient for a fixed magnetic quantum number m. The above formula for the linear conductance is specific for systems that confine electrons in two spatial directions [14].

3 Nanowire with a constriction: a cylindrical quantum point contact

We consider a nanowire with radius of $R = 5$ nm that contains a constriction of width $b = 8$ nm, whose radius R' can be controlled electrostatically by a gate voltage V_G, see Fig. 2. We model the constriction with a very high rectangular potential barrier, i.e. $V = 10$ eV. We consider for our modeling a scattering region of $2d_z = 32$ nm and an effective mass $m^* = 0.19m_0$.

The total tunneling coefficient $T^{(m)}$ as a function of the total energy E of the incident electron for two quantum numbers $m = 0$ and $m = \pm 1$ are presented in Fig. 3. Without constriction, i.e. $R = R'$, the tunneling coefficient increases with one each time the total energy reaches the energy of a transversal energy channel in the leads $E^{(m)}_{\perp,n}$, indicated by vertical dot-dashed lines. The tunneling coefficient for a fixed m shows deviations from this staircase characteristic when a constriction appears. Due to the supplemental confinement in the constriction region, $R' < R$, an effective one-dimensional barrier of the height $V^{(m)}_n$ appears for every transport channel n. So, the tunneling coefficient for every channel n, i.e. $T^{(m)}_{nn}$ takes values close to one only for energies higher than $V^{(m)}_n$. A good approximation for the height of this effective one-dimensional barrier is $V^{(m)}_n \simeq E'^{(m)}_{\perp,n} - E^{(m)}_{\perp,n}$, where $E'^{(m)}_{\perp,n}$ is the energy of the mode n in a infinitely long cylinder of radius R', see Eq. (5). So, the jumps appear approximately at $E'^{(m)}_{\perp,n}$, i.e. the energy channels in the constriction, indicated with dotted vertical lines. At higher energies this approximation breaks down, due to the finite length of the constriction. Based on this approximation, one can also understand the energy intervals between the steps. Those intervals increase quadratically with the energy due to the hard-wall lateral confinement that we have considered. In turn, decreasing the radius of the confinement, the plateaus will become longer. It is also clear, by comparing the plots in Fig. 3 that the positions and the lengths of the plateaus depend on the magnetic quantum number m through $E'^{(m)}_{\perp,n}$.

Furthermore, a resonant structure appears superimposed on the staircase characteristic. The tunneling coefficient for every channel n, i.e. $T^{(m)}_{nn}$, behaves like in the one-dimensional case, i.e. for energies above the barrier appear oscillations due to the Fabry-Pérot resonances [5, 53, 10]. The tunneling peaks arise from the interference effects

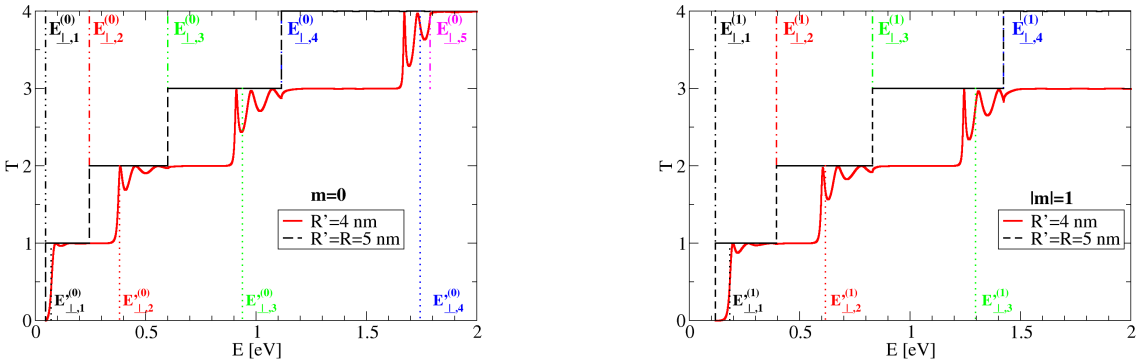


Figure 3: Tunneling coefficient $T^{(m)}$ versus total energy E of an incident electron for a nanowire with a constriction with $R' = 4$ nm and for magnetic quantum numbers $m = 0$ and $m = \pm 1$.

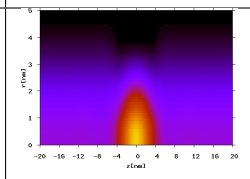
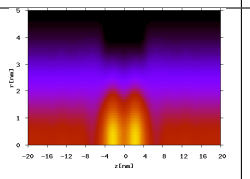
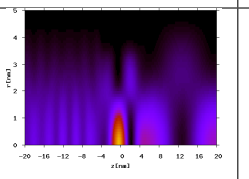
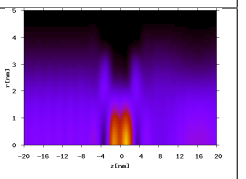
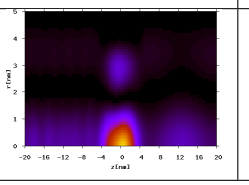
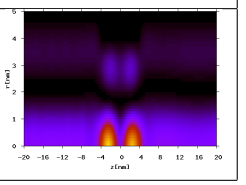
$m = 0$	$E = 0.092$ eV	$E = 0.159$ eV	$E = 0.384$ eV	$E = 0.453$ eV
$n = 1$				
$n = 2$				

Table 1: The localization probabilities $|\psi^{(s)}_{nm}(E; z, r)|^2$ in the domain $z \in [-20, 20]$ nm and $r \in [0, 5]$ nm for the resonant energies in Fig. 3 for $m = 0$. Bright colors mean high values.

between forward and backward propagation of electrons in the constriction region. The resonances become more obvious for higher plateaus, because the height of the effective barrier $V_n^{(m)}$ increases with the channel index n. The energy of these resonances can be approximated as the energy levels in a rectangular infinite potential well of width b, i.e. $E^{(m)}_{FP,i} - E'^{(m)}_{\perp,n} \propto (\hbar^2/2m^*)(i/b)^2$, where i is the order of the Fabry-Pérot resonance.

The localization probabilities $|\psi^{(s)}_{nm}(E; z, r)|^2$ of the electrons incident from source ($s = 1$) are represented as color maps in Table 1 for the resonant energies that appear in the tunneling coefficient in Fig. 3 for $m = 0$. Bright colors mean high values. As one can see, for the first two energies, $E = 0.092$ eV and $E = 0.159$ eV, there is a maximum of the localization inside the constriction, i.e. $(z, r) \in [-4, 4] \times [0, 4]$ and the number of the nodes in the z-direction corresponds to the order of the Fabry-Pérot resonance. For the next two energies, $E = 0.384$ eV and $E = 0.453$ eV the second energy channel inside the nanowire gets also open. For the electrons propagating within this channel, i.e. $n = 2$, the localization probabilities have a maximum inside the constriction and show a resonant behavior, i.e there is a clear zero node in the r-direction. For the electrons with

the same energy, but propagating within the first channel, i.e. $n = 1$, the localization probability does not show a resonant behavior, although there is a maximum inside the constriction. In conclusion, for every Fabry-Pérot type resonant peak in the transmission, only one wave function shows a resonant behavior, namely that of the last propagating channel [5, 55].

These results for a one-dimensional electron gas with a cylindrical constriction are to be expected, because they are similar to the quantization of the conductance in a cylindrically symmetric quantum point contact [6, 14]. It is clear that using the conductance formula (6) and considering that every magnetic quantum number m different from zero is double degenerated, see Eq. (3), one obtains in the conductance the quantized values $2e^2/h$ in the sequence $1, 3, 5, 6, 8, 10, ...$ [13], as presented in Fig. 1(b).

4 Nanowire with two constrictions. A cylindrical quantum point contact with an attractive potential

We consider now the same nanowire with two constrictions as in Fig. 2. For simplicity, the constrictions are considered identical of length $b_1 = b_2 = 8$ nm and of radius R', that can be varied continuously by an external gate voltage. The distance between the constrictions is $w = 8$ nm. Of course, in order to remain in the coherent ballistic transport regime, the geometrical dimensions of the constrictions and the distance between them have to be smaller than the elastic mean free path of the conduction electrons. We model again the constrictions by high rectangular barriers, i.e. $V = 10$ eV. We also consider the total length of the scattering region $2d_z = 32$ nm. The scattering potential is in this case not separable, so it mixes the energy channels n. Nevertheless, it produces conductance quantization, too [8].

The idea of considering systems with two or more quantum point contacts was followed by many research groups. Shortly after the first experiments on the quantum point contact [2], the same group has measured the conductance of a double-split-gate structure, i.e. two quantum point contacts in series [29]. For this structure an anomalous resistance due to the 2DEG wide region between the quantum point contacts alters the conductance quantization. The realization of two quantum point contacts in series on a nanowire will eliminate this anomalous resistance. Another configuration of two adjacent quantum point contacts in 2DEG was also used for studying the solid-state electron optics [11, 6]. The idea to consider a sequence of two constrictions along a quantum wire was also exploited in the realization of single-electron transistors [56, 57, 58]. But in these systems the active region is between the constrictions and consists in fact of a quantum dot that is studied. The gate that is changed in the conductance measurements controls mainly the number of the electrons inside the quantum dot, by changing the confining potential, i.e. changing its shape. In the first experiments the gate controls simultaneously the constrictions [56, 57] while in the other experiments the constrictions are kept by another gates at specified values, defining in such a way the coupling between the quantum dot and the reservoirs [58]. In the configuration proposed here, the nanowire plays a key role

providing the confinement of the carriers in two directions without supplemental gates, so that it offers a unique opportunity for the study of the ballistic conductance through two quantum point contacts in series.

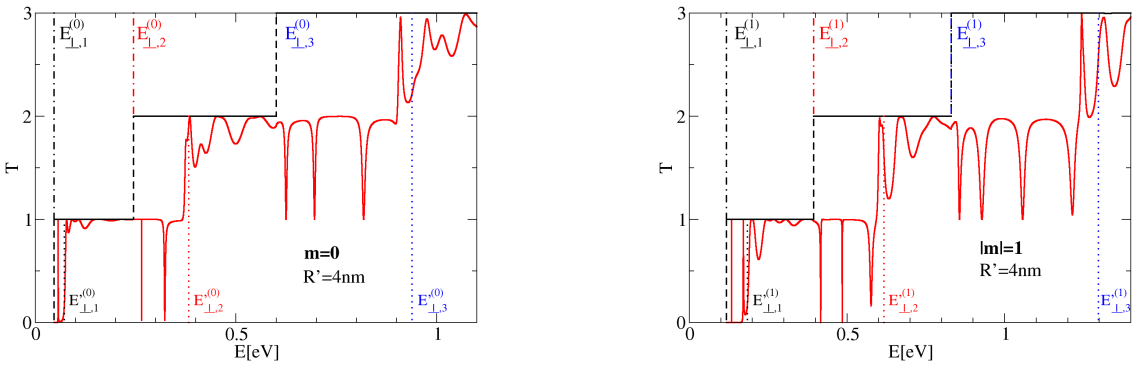


Figure 4: Tunneling coefficient $T^{(m)}$ versus total energy E of an incident electron for a nanowire with two constrictions with $R' = 4$ nm.

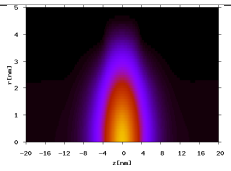
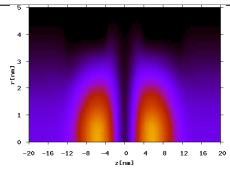
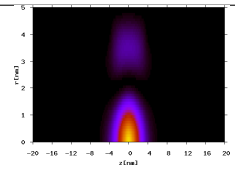
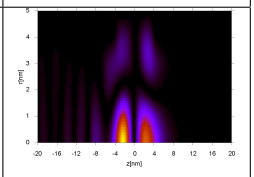
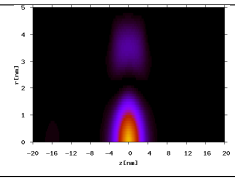
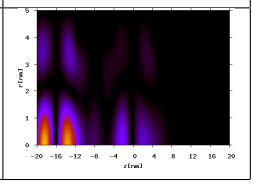
The total tunneling coefficient $T^{(m)}(E)$ for this structure is presented in Fig. 4 for two different values of the magnetic quantum number $m = 0$ and $m = \pm 1$. One can recognize the staircase structure of the tunneling coefficient, but there are clear tunneling peaks and dips. The vertical lines have the same meanings as in Fig. 3.

In order to understand the physical meaning of these peaks and dips, we will analyze the localization probabilities $|\psi^{(s)}_{nm}(E; z, r)|^2$ for the electrons with these energies incident from the source, presented in Table 2. The energy of the first resonance $E = 0.057$ eV is located between $E^{(0)}_{\perp,1}$ and $E'^{(0)}_{\perp,1}$. The localization probability for this energy has a pronounced maximum between the constrictions, i.e. $(z, r) \in [-4, 4] \times [0, 5]$ nm. For this energy, only one energy channels is open, so that a simple picture of non-mixing transmission channels can be applied. In turn, the two constrictions yield an effective double-barrier potential for the propagation within the energy channel n. The double-barrier potential yields resonances, that appear as tunneling peaks for energies below the height of the effective barrier $V^{(m)}_n$. This peak is very similar to the peak obtained by McEuen [48] and interpreted in terms of a hydrogenic donor atom. The position of this resonance with respect to the first energy channel in the nanowire can be also approximated as the lowest energy level in a rectangular infinite well of width w, so that $E^{(m)}_{\rm res} - E^{(m)}_{\perp,1} \propto (\hbar^2/2m^*)(1/w)^2$. The number of the resonant peaks can increase with m due to the increase of the effective potential barriers $V^{(m)}_n$. These resonances do not appear for higher quantization plateaus because of the non-separability of the scattering potential.

The next resonant energy $E = 0.078$ eV is greater than $E'^{(0)}_{\perp,1}$, and the localization probability shows two pronounced maxima over the regions of the constrictions, $z \in [-12, -4] \cup [4, 12]$ nm and $r \in [0, 4]$ nm. This is a Fabry-Pérot type resonance and its energy with respect to first energy channel in the constriction is set up by $1/b$, i.e. $E^{(m)}_{\rm FP,1} - E'^{(m)}_{\perp,1} \propto (\hbar^2/2m^*)(1/b)^2$.

For the next two resonances $E = 0.264$ eV and $E = 0.332$ eV that correspond to the

first two dips in the tunneling coefficient there are two energy channels open in the nanowire, i.e. $n = 1$ and $n = 2$. The localization probabilities for the electrons with these energies show maxima between the constrictions, i.e. $z \in [4, 4]$ nm and $r \in [0, 5]$ nm for both channels. This is a difference to the Fabry-Pérot type resonances, where only one energy channel provides the resonances.

$m = 0$	$E = 0.057$ eV	$E = 0.078$ eV	$E = 0.264$ eV	$E = 0.332$ eV
$n = 1$				
$n = 2$				

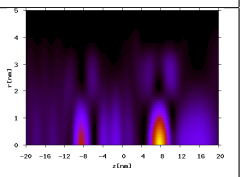
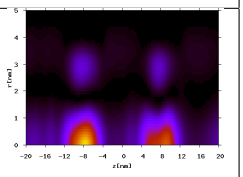
$m = 0$	$E = 0.384$ eV
$n = 1$	
$n = 2$	

Table 2: The localization probabilities $|\psi^{(s)}_{nm}(E; z, r)|^2$ in the domain $z \in [-20, 20]$ nm and $r \in [0, 5]$ nm for the energies of the peaks and dips in the tunneling coefficient from 4 of a nanowire with two constrictions for $m = 0$.

The energies of the dips are always between $[E^{(m)}_{\perp,n}, E'^{(m)}_{\perp,n}]$, so that the channel n is not yet open in the constrictions. We interprete these resonances as quasi-bound states of the evanescent channels inside the constrictions [34]. It was shown that an attractive scattering potential either in a quantum wire [39, 40, 41, 36, 42, 43] or in a nanowire [34] yields quasi-bound states of evanescent channels that appear as dips in the transmission coefficient. Both constrictions play the role of only one quantum point contact between the two reservoirs, and the piece of the nanowire between the constrictions plays the role of an effective attractive potential, because the transversal energy channels inside this region are lower than inside the constrictions. This interpretation is sustained also by the fact that the localization probabilities for both channels, i.e. $n = 1$ and $n = 2$, show a similar structure in the region between the constrictions. Both open channels in the nanowire propagate through the constrictions as an effective quantum point contact using the first open channel in the constrictions, but at those specific energies they reach the quasi-bound states of the second (evanescent) channel inside the constrictions. For

these quasi-bound states a back resonant reflection appears for both open channels. The number of nodes in the r-direction gives the information about the evanescent channel inside the constrictions. There is one node in the r-direction for both energies indicating that the second energy channel in the constrictions is used. The number of the nodes in the z-direction gives the order of the quasi-bound states of the evanescent channel. For the first dip there is no node in the z direction for $z \in [-4, 4]$ nm, while for the second dip there is one node in the z direction. The dips are well-separated from the subband $E'^{(0)}_{\perp,2}$, so that the localization probabilities do not extend much over the region between the constrictions. A characteristic of the quasi-bound states of the evanescent channels is that their localizations extend much more over the region of the attractive potential [34]. The energetical position of the dip i with respect to the evanescent subband $E'^{(m)}_{\perp,n}$

$$\Delta_i \propto \frac{\hbar^2}{2m^*}\left[x^2_{mn}\left(\frac{1}{R'^2}-\frac{1}{R^2}\right)-\frac{i^2}{w^2}\right] \tag{7}$$

is determined by the geometrical parameters R, R' and w. In such a way, the conductance of a quantum point contact with an attractive impurity is not independent on the quantum point contact length. In our case, the length of the effective quantum point contact is $b_1 + b_2 + w$.

At the next energy, $E = 0.384$ eV, the localization probabilities differ for the energy channels $n = 1$ and $n = 2$. Only the localization probability for the second channel shows a resonant structure inside the constrictions, while the propagation of the electron on the first energy channel is not resonant. We interprete this energy as a Fabry-Pérot type resonance of the second energy channel. The node in the r-direction shows a clear evidence of the second energy channel in the nanowire that is converted also to the second energy channel in the constrictions.

Quantum point contacts with impurities were subjects of theoretical [44, 45, 46, 47] as well as of experimental studies [48, 49, 50, 51, 52]. Especially, in the last decade a new technique was developed in order to study single quantum dots. Quantum point contacts are defined by lithography with an atomic force microscope and subsequent wet-chemical etching, such that one quantum dot is contained within the lithographically defined constriction [59, 49, 50, 52] The conductance resonances in Fig. 5 in Ref. [50] could be interpreted as signature of quasi-bound states due to the evanescent channels. This interpretation has to be treated with care because of the complexity of the structure. In Ref. [48] it is shown that a peak in the quantized conductance can appear before the turn-on of the first transverse mode, just similar with our result in Fig. 4. This peak is interpreted in terms of an unwanted and uncontrollable "hydrogenic" donor atom.

As one can see, the experimental realizations of quantum point contacts with impurities, especially attractive impurities, introduce unwanted effects produced by supplemental features of the system, i.e. supplemental gates in order to confine the region between the quantum point contacts or supplemental self-organized quantum dots that also influence the wide regions of the 2DEG, such that the interpretation of the measured conductance is not straightforward. The nanowire with two constrictions is a much simpler structure that could offer an ideal system for studying the quasi-bound states of the evanescent

channels. The effective attractive potential is provided by the nanowire itself and the transport is coherent through two quantum point contacts in series. Of course, the region of the nanowire between the two constrictions can be regarded as a quantum dot. The difference to the single-electron transistor studies [56, 57, 58] is that the gate voltage does not change the alignment of the energy levels of the quantum dot with respect to the Fermi level, but the widths of the quantum point contacts.

We present in Fig. 5 a comparison between the tunneling coefficients for a cylindrical nanowire with a constriction and with two constrictions for the first two subbands for a fixed magnetic quantum number m. The vertical dashed and dotted lines have the same meanings as in Fig. 3. The influences of the geometrical parameters R, R', b and w on the resonant energies are also schematically indicated.

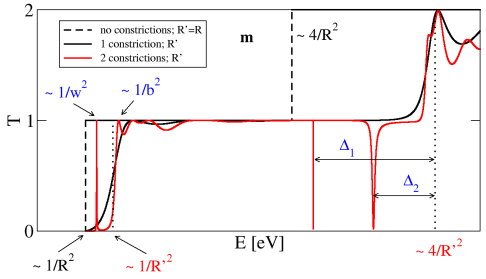


Figure 5: Tunneling coefficient $T^{(m)}$ for a cylindrical nanowire with one or two constrictions, for a specific magnetic quantum number m. The influences of the geometrical parameters on the resonant energies are also shown.

5 Conclusions

We have studied a one-dimensional electron gas, i.e. cylindrical semiconductor nanowire, with one or two constrictions. Following the Landauer formula, the linear conductance at low temperature is given by the total tunneling coefficient at the Fermi energy. Using the R-matrix formalism, we have computed the energy dependence of the tunneling coefficient for both systems. Representing the localization probabilities at the resonant energies we could identify the physical meaning of them. It was shown that the nanowire with two constrictions yields a very simple and accurate system for the experimental evidence of the quasi-bound states of the evanescent channels. These quasi-bound states provide dips in the tunneling coefficient, an effect very well-known theoretically but not yet evidenced experimentally. Many experiments for quantum point contacts with impurities in 2DEG show deviations from the clear conductance quantization, that give hints to the existence of these quasi-bound states.

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