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Conductance oscillations of a quantum wire disturbed by an adatom

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Abstract

The conductance through a quantum wire with a side-attached atom (adatom) is investigated using the tight-binding Hamiltonian and Green function method. The adatom can be coupled with one or more atoms and it disturbs the electron transport through the wire. Analytical formulae for the transmittance are obtained for the most probable connections. Also, conductance oscillations as a function of the wire length are studied for a disturbed wire. It is shown that the period of these oscillations remains unchanged in the presence of the adatom but the value of the conductance strongly depends on the adatom–wire couplings and the kind of connections of the adatom to the wire.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The physics of one-dimensional structures has been the focus of experimental and theoretical studies generally due to their potential applications in electronics. Monoatomic quantum chains are the thinnest possible electrical wires. Such structures can be investigated experimentally, for example by using the mechanically controlled break junction (MCBJ) [1, 2] or scanning tunnelling microscope (STM) technique [3]. Very long and well ordered gold wires (single or double) can also be fabricated on silicon vicinal surfaces; see e.g. [4–6].

It was shown experimentally [1] and confirmed theoretically [7–11] that for an odd (even) number of atoms in a chain the conductance is maximal (minimal). This effect, known as the even–odd conductance oscillations, is satisfied when the single particle energies of quantum wire (QW) atoms correspond to the Fermi energy of the system and can be explained for example in terms of charge neutrality [7]. Also, oscillations with a period greater than two are possible, and they have been predicted theoretically [12–15]. The main reason for these oscillations is the interference effect between the electron Fermi wavelength and the chain length [12], which leads to different chain filling factors [14, 15].

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The electronic properties of one-dimensional structures are modified by side-attached atoms. The problem of impurities (atoms, quantum dots, chemical compounds) in monoatomic chains has been studied both theoretically, see e.g. [16–23] and experimentally, see e.g. [24–29]. Density-functional theory (DFT) studies show that a H_2 molecule incorporated in a gold wire (between QW atoms) is a robust configuration, which can be reached without any barrier [16]. In this case the conductance decreases because electrons must flow through the impurity which is between QW atoms. For an impurity localized at the wire side the electrons can flow directly through the wire or through the impurity (depending on the QW–impurity connection). In that case the conductance can increase or decrease due to interference effects. The above-mentioned theoretical papers have not considered the conductance oscillations of a wire with a side-attached adatom, coupled in different ways to the wire.

The MCBJ experiments [25–27] and DFT calculations [16] show that the hydrogen (or oxygen) molecules are placed between wire atoms; thus the chain of Au atoms can be pulled in this environment. Moreover, the conductance of such a disturbed wire decreases to a fractional value but is characterized by a periodic behaviour as a function of the wire length [27]. These oscillations are very similar to the even–odd conductance oscillations but they are modified by various configurations (orientation) of the H_2 molecule incorporated in the gold wire.

In this paper we study the influence of a side-attached adatom on the conductance through a monoatomic wire. It is a very interesting and important problem to know what modifications of the conductance one can expect in the case when a wire is disturbed by a side-attached adatom. The adatom can be described by the same (different) parameters as the wire atoms, i.e. the wire and the adatom are composed of the same (different) material. Moreover, the adatom can be coupled with only one QW atom (one-to-one connection), with two (one-to-two connection) or with more QW atoms. Starting from the tight-binding Hamiltonian and using a Green function formalism, the zero-temperature conductance is obtained (see e.g. [11, 14, 30–34]) and analytical formulae are shown for the most probably connections. We will mostly concentrate on studying the conductance oscillations in a wire disturbed by an adatom.

The model we consider here can be realized experimentally. It is known that one-dimensional monoatomic gold wires can be observed on vicinal silicon surfaces; see e.g. [4–6]. On such a prepared chain, using the epitaxy method or STM manipulation, one can put another atom (adatom) on the wire. It can be metallic, semiconducting or other form of adatom. This adatom, depending on its position with respect to QW atoms, can be coupled with one or more QW atoms. Also, one can change the coupling strength between the adatom and the QW atoms (it depends on the distance between atoms). To measure the conductance through such a disturbed wire, two electrodes are needed. One of them is the STM tip, and the second electrode can be made for example by an epitaxy method. By changing the position of the STM tip over the wire the current can flow through various numbers of atoms in the wire (between two electrodes) and the conductance measurement is possible. The influence of the Si surface on the conductance between these two electrodes can be eliminated in a low-temperature regime as there is an energy gap in semiconductor materials. The value of the single-particle energy of the QW atoms can be changed by applying a potential to the surface. Of course one can also consider a second realization of this system, i.e. the case of two bulk electrodes (or metallic islands) on the surface connected by a monoatomic wire to an adatom deposited near the wire (in that case the number of atoms between electrodes remains constant). By using, for example, STM manipulation of the adatom on such a surface, one may change the current flowing through the wire (between electrodes) in a controllable way because it is possible to move the adatom along the wire and thus change the adatom–QW atoms connection. Such manipulation of the adatom versus the QW atoms cannot be done in the arbitrary way as it depends on the surface atoms' positions (there are preferable sites for the adatom on the

surface). But moving the adatom between two surface sites (which are localized near the wire) one can change or block the current flowing through the wire. This can be a very useful effect when considering two nanodevices (e.g. logic gates, qubits, transistors) which are connected via the thinnest possible electric wire, i.e. a monoatomic quantum wire. Such devices must exchange information between each other and thus the electric state of the wire is crucial for the operating process. The system of a wire with an adatom can also be considered as an element of a nanotransistor because the current flowing through such a device can be controlled by the adatom position versus the wire atoms. MCBJ experiments cannot control the process of adsorbing additional atoms on the wire. Moreover, such atoms are incorporated between wire atoms, and thus disturb the main tunnelling channel [24–29]. Of course, using the MCBJ method the adatom can join to the wire, but there are no experimental instruments to indicate the position and kind of connection of such an adatom. Moreover, one cannot control the number of adatoms which are adsorbed onto the wire.

The paper is organized as follows. In section 2 the model and formalism are presented. Also analytical formulae for the transmittance are obtained. Numerical results are shown and discussed in section 3. The main conclusions of this paper are presented in section 4.

2. Model and formalism

The system of a quantum wire with a side-attached adatom can be described by the following Hamiltonian: $H = H_{\mathrm{wire}} + H_{\mathrm{adatom}}$, where $H_{\mathrm{wire(adatom)}}$ concerns the wire (adatom) energy (the nearest-neighbour interactions are assumed), and can be written in the form

$$H_{\mathrm{wire}} = \sum_{\vec{k}\alpha=\mathrm{L,R}} \varepsilon_{\vec{k}\alpha} a^{\dagger}_{\vec{k}\alpha} a_{\vec{k}\alpha} + \sum_{i=1}^{N} \varepsilon_i a^{\dagger}_i a_i + \sum_{\vec{k}\mathrm{L},\vec{k}\mathrm{R}} V_{\vec{k}\mathrm{L(R)}} a^{\dagger}_{\vec{k}\mathrm{L(R)}} a_{1(N)} + \sum_{i=1}^{N-1} V_i a^{\dagger}_i a_{i+1} + \mathrm{h.c.} \qquad (1)$$

and

$$H_{\mathrm{adatom}} = \varepsilon_x c^{\dagger}_x c_x + \sum_{i=1}^{N} t_i c^{\dagger}_x a_i + \mathrm{h.c.}$$

Here, the operators $a_{\vec{k}\alpha}(a^{\dagger}_{\vec{k}\alpha})$, $a_i(a^{\dagger}_i)$ and $c_x(c^{\dagger}_x)$ are the electron annihilation (creation) operators in the lead α ($\alpha = \mathrm{L, R}$), at the atomic site i ($i = 1, \ldots, N$) and at the adatom, respectively. The element $V_{\vec{k}\mathrm{L(R)}}$ is the electron tunnelling coupling (hopping integral) between the states in the left (right) reservoir and the first (last) atom and V_i is the tunnelling coupling between the electron states of the ith and $(i + 1)$th atoms. The element t_i corresponds to hybridization between the adatom and quantum wire states. The system we consider here is shown in figure 1(a). In figures 1(b)–(d) the possible connections of the adatom to the QW are visible; these are discussed later.

The electron spin index in the Hamiltonian is suppressed and the electron–electron correlations are neglected in the first step as we consider here only paramagnetic solution, and the adatom is not a magnetic one. The model described here can be applied to systems where the interaction energy is smaller than the kinetic energy associated with hopping integrals between QW atoms (e.g. Au chains on vicinal silicon surfaces where the correlation effects are negligible due to small carrier concentration). In such a system many-body effects can be neglected. It is known that the Coulomb interaction does not change the conductance oscillations in the case when the QW energy levels correspond to the Fermi energy, E_{F}. In general, the electron–electron correlations act as an additional scattering mechanism, and they can change only the value of the conductance (monotonically with N) and thus do not change the period of the conductance oscillations [15, 35, 36]. Also, a side-attached impurity with

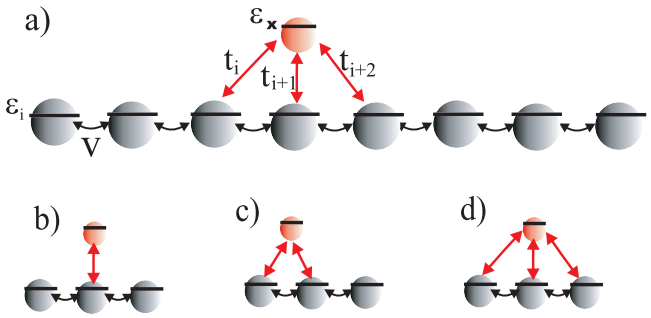

Figure 1. A schematic view of the considered systems: (a) quantum wire with side-attached adatom and (b)–(d) different connections of an adatom to the wire.

strong electron–electron interaction reduces the conductance [17, 18]. The on-site Coulomb interaction introduces a renormalization of the site energies (when we are not interested in, for example, the Kondo effect) and one can expect that the general results of this paper remain valid for non-magnetic atoms; see also [23].

The linear conductance at zero temperature is proportional to the total transmittance and satisfies the Landauer formula [30–34]: $G(E_{\mathrm{F}}) = \frac{2e^2}{h}T(E_{\mathrm{F}})$. The transmittance depends on the Fermi energy of the system and in our case can be found from the formula $T_N(\varepsilon) = \Gamma^{\mathrm{L}}\Gamma^{\mathrm{R}}|G^{\mathrm{r}}_{1N}(\varepsilon)|^2$, where G^{r} is the retarded Green function (obtained using the equation of motion for the retarded Green function) which refers to the two ends of the wire and $\Gamma^{\mathrm{L/R}} = 2\pi \sum_{\vec{k}\mathrm{L/R}} V_{\vec{k}\mathrm{L/R}} V^*_{\vec{k}\mathrm{L/R}} \delta(\varepsilon - \varepsilon_{\vec{k}\mathrm{L/R}})$. The general matrix equation for the retarded Green function $G^{\mathrm{r}} = (G^{\mathrm{r}})_{i+1,j+1}$ $(i, j = 1, \ldots, N)$ can be written in the form

$$\tilde{A} \cdot G^{\mathrm{r}} = \begin{pmatrix} A^N & \tilde{t}^T \\ \tilde{t} & \varepsilon - \varepsilon_x \end{pmatrix} \cdot G^{\mathrm{r}} = I \tag{2}$$

where I is the unit matrix, $\tilde{t}$ is the vector describing the adatom–QW couplings (in general the adatom can be coupled with all QW atoms), $\tilde{t} = -(t_1, t_2, \ldots, t_N)$, and A^N is the matrix which corresponds to the wire without the adatom (non-disturbed wire), i.e.

$$A^N = A^N_{ij} = (\varepsilon - \varepsilon_i)\delta_{i,j} - V_i(\delta_{i,j+1} + \delta_{i+1,j}) + \mathrm{i}\frac{\Gamma}{2}(\delta_{i,1}\delta_{1,j} + \delta_{i,N}\delta_{N,j}). \tag{3}$$

The retarded Green function G^{r}_{1N} is obtained by finding the inverse of the matrix $\tilde{A}$. To obtain the analytical relation for the conductance we assume the same electron energies of all atoms in the wire, i.e. $\varepsilon_i = \varepsilon_0$, and the same coupling strength between the nearest-neighbour electron states in the wire, $V_i = V$. Moreover, we consider the symmetric case $\Gamma^{\mathrm{L}} = \Gamma^{\mathrm{R}} = \Gamma$. In real physical systems an adatom can be coupled with only a few QW atoms. The most probable configurations are: one-to-one connection (see figure 1(b)) or one-to-two connection (see figure 1(c)). The configuration presented in figure 1(d) can be considered as a modification of the one-to-one or one-to-two connections. For our purposes, we mainly concentrate on the two configurations shown in figures 1(b) and (c).

In the first step we consider an adatom coupled with only one QW atom, i.e. $\tilde{t} = (0, \ldots, -t_m, \ldots, 0)$, $(m = 1, \ldots, N)$; see figure 1(b). Here the adatom is coupled with the mth atom of the wire, and in this case the transmittance can be expressed as follows:

$$T_N = \frac{\Gamma^2 V^{2(N-1)}}{|\det(A^N) - \frac{t_m^2}{\varepsilon - \varepsilon_x}\det(B^{m-1})\det(B^{N-m})|^2} \tag{4}$$

where $\det A^N$ can be obtained from the relation $\det(A^N) = \det(A_0^N) + \mathrm{i}\Gamma \det(A_0^{N-1}) - (\frac{\Gamma}{2})^2 \det(A_0^{N-2})$, and $\det(B^k)$ is the determinant of the matrix which can be expressed as $\det(B^k) = \det(A_0^k) + \mathrm{i}\frac{\Gamma}{2}\det(A_0^{k-1})$, with the conditions $\det(A_0^{-1}) = 0$, $\det(A_0^0) = 1$ and $\det(A_0^1) = \varepsilon - \varepsilon_0$. The determinant $\det(A_0^k)$ corresponds to a quantum wire that is not coupled to the leads and is not disturbed by the adatom, and in our case it can be obtained fully analytically, i.e. $\det(A_0^k) = V^k u_k(\phi)$, where $u(\phi)$ is a Chebyshev polynomial of the second kind and ϕ plays the role of the Bloch phase $\phi = \arccos(\frac{\varepsilon - \varepsilon_0}{2V})$.

Next we consider an adatom coupled with the mth and $(m+1)$th QW atoms, i.e. $\tilde{t} = (0, \ldots, -t_m, -t_{m+1}, \ldots, 0)$, which corresponds to the case shown in figure 1(c). Here we assume that the adatom is placed between QW atoms and $t_m = t_{m+1} = t$. In this case the transmittance can be written in the form

$$T_N = \Gamma^2 V^{2(N-2)} \left(V + \frac{t^2}{\varepsilon - \varepsilon_x} \right)^2 \left\{ \left| \det(A^N) - \frac{t^2}{\varepsilon - \varepsilon_x} [2V \det(B^{m-1}) \det(B^{N-m-1}) + \det(B^{m-1}) \det(B^{N-m}) + \det(B^m) \det(B^{N-m-1})] \right|^2 \right\}^{-1}. \quad (5)$$

For a non-disturbed QW, $t = 0$, the above relation (and also equation (4) for $t_m = 0$) can be simplified, i.e., $T_N = \Gamma^2 V^{2(N-1)} / |\det(A^N)|^2$. One can obtain a more complicated expression for the case when the adatom is coupled with three QW atoms. In this case or in general when the adatom is coupled with many QW atoms the transmittance should be obtained numerically.

Equations (4) and (5) are the general analytical formulae for the transmittance of a wire with a side-attached adatom. These relations are valid for arbitrary length of the wire and are the main formulae of this paper.

3. Results and discussion

Next we investigate the conductance of a wire with a side-attached adatom as a function of the wire length. It is known that for certain values of the single-electron energies in the wire, ε_0, the conductance oscillates with the length of the wire. For the case when ε_0 corresponds to the Fermi energy, even–odd conductance oscillations can be observed. Also, conductance oscillations with a period larger than two can be observed, see e.g. [12–15], and the general condition for these oscillations has been obtained [14]. In the presence of a side-attached adatom these oscillations depend on the adatom parameters and its connection to the wire.

In our calculation we express all energies in units of Γ. The other parameters have been chosen in order to satisfy the real STM experiments, and for example taking $\Gamma = 0.04$ eV we get $V = 0.16$ eV and the parameters t_i between 0 and 0.16 eV. First let us analyse the even–odd conductance oscillations case, i.e. $\varepsilon_0 = E_\mathrm{F} = 0$. In figure 2, the conductance (in $2e^2/h$ units) is shown as a function of the wire length and for various adatom–QW atom connections. In the upper panel the adatom is connected to the first QW atom. For $t_1 = 0$ the conductance oscillations with a period of two are visible as a function of N (alternately white or black colours). In the presence of the adatom, $t_1 > 0$, these oscillations disappear—the maximal conductance for the odd-length wire decreases with t_1 and for the even-length wire the conductance is minimal and remains almost unchanged. For the adatom connected to the second QW atom ($t_1 = 0, t_2 \neq 0$—not shown here) we obtain very similar results to those shown in figure 1 (upper panel): the only difference is that the conductance decreases more slowly with t_2 in comparison to the first QW atom connection. Generally, for an adatom connected to every odd-atom in the wire (i.e. to the first, third, fifth atom) we obtain the result as for the connection to the first QW atom. For the connection to every

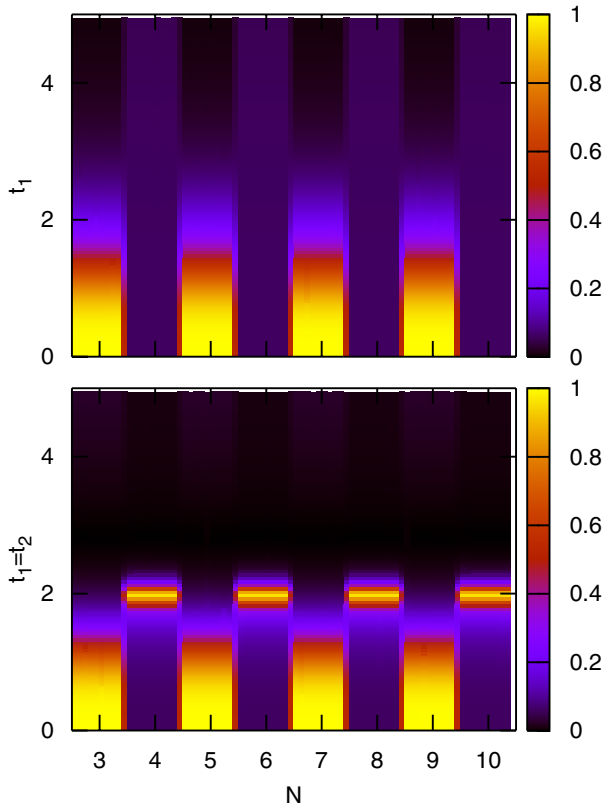

Figure 2. The conductance (in $2e^2/h$ units) for the even–odd oscillation, $\varepsilon_0 = 0$, versus the length of a wire and for one-to-one connection t_1 (upper panel) and for one-to-two connection $t_1 = t_2$ (lower panel); $\varepsilon_x = 2$, $V = 4$. All energies are expressed in units of Γ.

even-atom in the wire (i.e. to the second, fourth, etc) the results are the same as for the connection to the second QW atom. This effect is due to the modification of the QW local density of states (LDOS). It is known that every odd (even) atom in non-disturbed wire is characterized by a maximum (minimum) value at the Fermi level. The adatom connected to the QW atom (one-to-one connection) causes the LDOS at the Fermi level to decrease, and thus the conductance also decreases. This can be also explained from equation (4), where for $\varepsilon_0 = E_F = 0$ the following relation is satisfied: $\det B^{i-1} \det B^{N-i} \equiv \det B^{(i+2)-1} \det B^{N-(i+2)}$; and in this case $T(i) = T(i+2)$, where the number i indicates the QW atom. The above conclusion is valid for $\varepsilon_x \neq 0$. For $\varepsilon_x = 0$ the conductance is blocked for all N (the determinant of equation (4) tends to infinity) and the conductance oscillations are not observed.

In the lower panel (figure 2) the adatom is connected to the first and the second QW atoms with the same coupling strength $t_1 = t_2 = t$ and the conductance is obtained from equation (5). Here we observe that for the odd-length wire the conductance decreases with t whereas for the even-length wire the conductance strongly depends on t and reaches the maximal value for $t \simeq V/2$. In this case, instead of even–odd conductance oscillations we obtain odd–even oscillations. Such an effect was not observed for the one-to-one connection. For a certain value of t or $t \gg 0$ the conductance does not oscillate, and it reaches a constant value for all N.

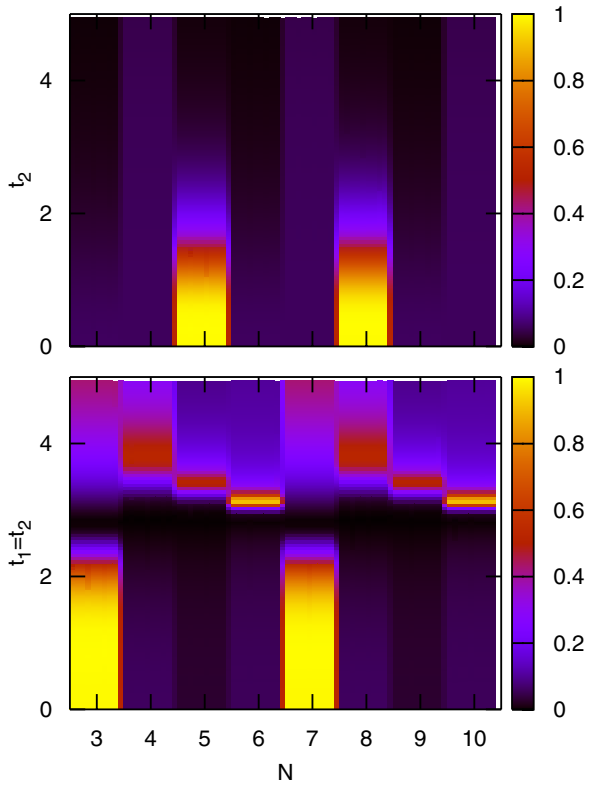

Figure 3. The conductance oscillations with period equal to three, $\varepsilon_0 = V$, and one-to-one connection as a function of t_2 (upper panel) and with period equal to four, $\varepsilon_0 = \sqrt{2}V$, and an adatom connected to two QW atoms $t_1 = t_2$ (lower panel); $\varepsilon_x = 2$, $V = 4$.

The suppression of the conductance for the one-to-one connection is due to the Fano interference between the ballistic wire channel and the adatom disturbance. On the other hand, for the one-to-two connection there are two ballistic channels—through the wire and through the adatom. The coupling strength between the wire and the adatom changes the probability for the path through the adatom and thus influences the probability for the path through the QW atoms. In this case the electron can interfere (destructively or constructively) and the conductance locally increases.

Next we consider the case when the on-site energies in the wire, ε_0, do not correspond to the Fermi energy of the system. In figure 3 we show the conductance oscillations for different connections of the adatom to the wire with periods equal to three and four. The upper panel corresponds to the one-to-one connection, $t_2 \neq 0$, with the condition $\varepsilon_0 = V$ (the condition for three-atom conductance oscillations [14]). For a small value of t_2 these oscillations are very well visible, but the conductance decreases, and for enough large t_2 the conductance is blocked for all N. This conclusion is valid for $\varepsilon_x \neq 0$ but one can also find regions where the conductance locally increases with t_2. This effect is due to shifting of ε_0 in comparison to the Fermi energy (the symmetry of the LDOS is broken). The lower panel in figure 3 shows the conductance oscillations for $\varepsilon_0 = \sqrt{2}V$ (the condition for a four-atom period [14]) for an adatom connected to two QW atoms, $t_1 = t_2 = t$, as a function of t. For small values of t

these oscillations are not disturbed. For a certain value of t the conductance is blocked for all N, which is a hallmark of a destructive interference effect. The interference effects which are visible in the lower panel in figure 3 are similar to those in figure 2.

We can see from figures 2 and 3 that the adatom does not change the period of the conductance oscillations. This effect can be shown from equations (4) and (5) by solving the relation $T_N = T_{N+l}$, where l is the period of the conductance oscillations. It is worth mentioning that the parameters which describe the adatom (i.e. t, ε_0) are not included in the determinants det A and det B, and thus the condition on the conductance oscillations remains the same as for non-disturbed wire. Moreover, the adatom only changes the conductance value depending on the kind and the strength of its connection to the wire, and it can change or reverse the maximal and minimal values. The explanation of this effect is rather simple. In this geometry the electron path through the QW atoms exists in the presence of the adatom and thus the main features of a non-disturbed wire can be still valid. This is the reason we observe conductance oscillations for a disturbed wire. Note that this conclusion may not be valid for the geometry when the adatom is incorporated between QW atoms.

4. Conclusions

In summary, using the tight-binding Hamiltonian and Green function method, the zero-temperature conductance through a quantum wire disturbed by a side-attached atom was investigated. The same couplings strength between the nearest-neighbour electron states in the wire and the same single-particle electron energies in the wire were assumed. The analytical formulae were derived for the most probable connections of the adatom to the wire, equation (4) (for one-to-one connection) and equation (5) (for one-to-two connection). These relations are valid for any QW length and for the adatom connected to any arbitrary QW atom. The main conclusion of this paper is that the adatom does not change the period of the conductance oscillations. This result is independent of the kind of adatom–QW atom connection. The conductance of the wire disturbed by the adatom can change only its value. This leads to the very interesting situation when, for example, instead of the even–odd conductance oscillations for a non-disturbed wire we get odd–even (or no) oscillations in the presence of the adatom; see figures 2 and 3. Moreover, it is worth noting that for the one-to-one connection the conductance decreases due to the disturbance of the ballistic channel (through the QW atoms) by the adatom. In the case when the adatom is coupled with two or more QW atoms the conductance can increase, which is a hallmark of the Fano effect.

The results of this paper were obtained for no electron–electron correlations (U) in the system, and thus describe materials where U is not important, like for example Au wires on vicinal Si surfaces [5, 6]. However, in the presence of on-site Coulomb interactions, additional approximations should be made to obtain the conductance of the system. Using the equation of motion for the retarded Green function, the most popular is decoupling of the high-order Green functions in the Hartree–Fock manner. This approximation, for the limit $U \to 0$, leads to the same results as for the system with no correlations. This means that for rather small U the result of this paper must be valid. In the case of large U, which describes for example ferromagnetic materials, one expects additional resonance peaks to appear in the local density of states (the peaks for $U = 0$ are split), and finally this leads to renormalization of the single-electron energy and can change the value of the conductance. Using the Dyson equation for the retarded Green function, the electron–electron correlations are included in the self-energy terms but also one should use additional approximations (e.g. a perturbation approach) to obtain the total Green function. In this case the Coulomb correlations just shift and split the conductance resonance position versus the energy [11]. It is worth noting that the conductance

oscillations effect appears for $U = 0$ and thus it is not necessary to include any type of electron correlations in the calculations. For ferromagnetic systems, for non-zero U, the conductance can change its value, see [15, 35, 36], but it is believed that the conclusions of this paper remain valid.

It is expected that these results can be confirmed experimentally, for example by using the STM method for wires on vicinal surfaces. The studies of such one-dimensional structures can be very useful for miniaturization of electrical wires or in nanotechnology.

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