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Abstract
The electron transport through a monatomic metallic wire connected to leads
is investigated using the tight-binding Hamiltonian and the Green function
technique. Analytical formulae for the transmittance are derived and M-atom
oscillations of the conductance versus the length of the wire are found. Maxima
of the transmittance function versus the energy, for a wire consisting of N atoms,
determine the $(N + 1)$ period of the conductance. The periods of conductance
oscillations are discussed and the local and average quantum wire charges are
presented. The average charge of the wire is linked with the period of the
conductance oscillations and for M-atom periodicity there are possible $(M - 1)$
average occupations of the wire states.

1. Introduction

The study of electron transport through mesoscopic systems is one of the most fundamental
theoretical and experimental problems in nanostructure physics. Interest in quantum transport
in low-dimensional systems has increased enormously during recent years due to its potential
applications in electronics and the very interesting and new phenomena we can investigate in
such structures.

The conductance of quantum wires has been investigated both experimentally and
theoretically by several authors. The experimental investigation of these structures requires
tools for manipulations of atoms at the nanoscale. One way of producing one-dimensional
materials of atoms is to grow them on metal surfaces [1–4]. Also, using a scanning tunnelling
microscope (STM) technique it is possible to fabricate a few-atom chain between the tip of
the STM and a metallic substrate; see for example [5]. To investigate the electron transport
through a monatomic quantum wire (QW) the mechanically controlled break junction (MCBJ)
method can be used as well [6–8].

The conductance of an atomic chain oscillates with a period of two atoms as the length
of the wire is changed. This effect is known as the even–odd conductance oscillation. Using

the Friedel sum rule, Sim *et al* [9] showed that for an odd number of atoms in the chain the conductance was maximal while for an even number of atoms the conductance was lower. These oscillations have been confirmed experimentally using the MCBJ method for Au, Pt and Ir atoms [6, 7]. The even–odd behaviour of the conductance can be understood in terms of the level-splitting in quantum physics and the particle–hole symmetry in the energy spectrum when all the QW energy levels lie at the Fermi energy of the system [10]. This symmetry is also visible in the transmittance function of the system or in the local density of states around the wire at the Fermi level [11, 12]. In this case the conductance can be expressed analytically; see for example [10, 13]. Also, calculations based on density functional theory for the conductance of the monatomic Al wires have shown the four-atom oscillations of the conductance [14]. This behaviour was explained by combining a resonant transport picture with the electron structure of the free atomic wire (not connected to electrodes). Thygesen and Jacobsen [14] also found that the period of oscillations is determined by the filling factor of the valence band of the infinite wire. In their calculations the half-filled band of the infinite wire implies even–odd oscillations while the filling factor of 0.25 leads to a four-atom periodicity.

The influence of external time-dependent fields on the conductance of a wire connected to leads was studied theoretically using the evolution operator technique [15]. Two regimes of frequencies of the external fields were distinguished and the six-atom period of the conductance was found. This period was explained in terms of the structure of the transmittance coefficient of the system. Using the Su–Schrieffer–Heeger type of Hamiltonian and the Green function technique, Onipko *et al* [16] have found a semi-analytical expression for the tunnel conductance for oligomers such as C_2H_2, C_2H_4S. However, the final result of this work does not describe any period of conductance oscillations.

The theoretical works mentioned above are based on numerical calculations and do not present analytical formulae of the conductance except the even–odd conductance oscillations. In this theoretical work we focus on the analytical solutions of the conductance of a metallic wire between two reservoirs. The tight-binding Hamiltonian and the Green function method are used in our calculations. Analytical expressions for the transmittance are obtained and the general condition on the conductance oscillations is found. Also the details of the conductance oscillations are discussed and the local and average charges of the wire are analysed.

The paper is arranged as follows. In section 2 the transmittance function for the various parameters describing the wire is obtained. In section 3 the general results (the conductance and the local and average QW charges versus the length of the wire) and discussion are presented. Conclusions are given in the last section.

2. Formalism and analytically solvable cases

In this section, the model and formalism are presented and analytical formulae allowing us to calculate the transmittance and the conductance of a wire are derived. The following notation is used in the paper: the capital letter N expresses the length of the wire while the capital letter M means the period of conductance oscillations.

The wire is modelled as a chain of atoms with its ends connected to the left and right leads by the following tight-binding Hamiltonian:

$$H = \sum_{\vec{k}\alpha=\text{L,R}} \varepsilon_{\vec{k}\alpha} a^{\dagger}_{\vec{k}\alpha} a_{\vec{k}\alpha} + \sum_{i=1}^{N} \varepsilon_i a^{\dagger}_i a_i + \sum_{\vec{k}\text{L},\vec{k}\text{R}} V_{\vec{k}\text{L(R)}} a^{\dagger}_{\vec{k}\text{L(R)}} a_{1(N)} + \sum_{i=1}^{N-1} t_i a^{\dagger}_i a_{i+1} + \text{h.c.} \tag{1}$$

where the operators $a_{\vec{k}\alpha}(a^{\dagger}_{\vec{k}\alpha})$, $a_i(a^{\dagger}_i)$ are the electron annihilation (creation) operators in the

lead α ($\alpha = $ L, R) and at atomic site i ($i = 1, \ldots, N$). The element $V_{\bar{k}L(R)}$ is the electron tunnelling coupling between the states in the left (right) reservoir and the first (last) atom and t_i is the tunnelling coupling between the electron states of ith and ($i + 1$)th atoms. The electron spin index is omitted and the electron–electron correlation is neglected in the first step as we concentrate on finding the general condition for conductance oscillations. For simplicity a single orbital per site and nearest-neighbour interactions only are assumed.

The conductance, in the linear response regime and at zero temperature, is simply proportional to the total transmittance: $G(E_F) = \frac{2e^2}{h}T(E_F)$. The transmittance depends on the Fermi energy of the system and in our case can be found from the formula [17]

$$T_N(E) = \text{Tr}\{\Gamma_L G^r \Gamma_R G^a\} = \Gamma^L \Gamma^R |G^r_{1N}(E)|^2, \tag{2}$$

where G^r (G^a) is the matrix of retarded (advanced) Green functions. The only nonzero element of the matrix Γ_L is $(\Gamma_L)_{11} = \Gamma^L$ and the function Γ^L is expressed as follows: $\Gamma^L = 2\pi \sum_{\bar{k}L} V_{\bar{k}L} V^*_{\bar{k}L} \delta(\varepsilon - \varepsilon_{\bar{k}L})$ (we can write a similar expression for Γ^R). To find the transmittance or conductance of the QW connected to the leads one needs to find the retarded Green function G^r_{1N} which refers to the two ends of the wire, equation (2). Using the equation of motion for the retarded Green function [17] and the Hamiltonian one can write the general matrix equation for G^r_{ij}, i.e. $A^N \cdot G^r = I$, where I is the unit matrix and

$$A^N \equiv A^N_{ij} = (E - \varepsilon_0)\delta_{i,j} - t_i(\delta_{i,j+1} + \delta_{i+1,j}) + i\frac{\Gamma}{2}(\delta_{i,1}\delta_{1,j} + \delta_{i,N}\delta_{N,j}), \tag{3}$$

where $i, j \leqslant N$ and A^N_{ij} is an $N \times N$ tridiagonal symmetric matrix. The retarded Green function G^r_{ij} is obtained by finding the inverse of the matrix A^N, i.e. $G^r = (A^N)^{-1}$. Here, we consider the symmetric case $\Gamma^L = \Gamma^R = \Gamma$ and assume the same electron energies of all atoms in the wire, i.e. $\varepsilon_i = \varepsilon_0$, and the same coupling strengths (hoppings) between the nearest-neighbour electron states in the wire, $t_i = t$. These are quite reasonable assumptions as we concentrate on the linear conductance (very small or zero source–drain voltage) and take into consideration a wire formed of the same atoms. In our calculations we put the Fermi energy as the reference energy point and obtain the transmittance for $E = E_F$.

To find the transmittance, equation (2), one has to obtain the Green function G^r_{1N}, which can be expressed, using equation (3), in the form

$$G^r_{1N} = \frac{(-t)^{N-1}}{\det(A^N)}. \tag{4}$$

The determinant of the matrix A^N satisfies the following relation:

$$\det(A^N) = \det(A^N_0) + i\Gamma \det(A^{N-1}_0) - \frac{\Gamma^2}{4}\det(A^{N-2}_0), \tag{5}$$

where A^N_0 is the matrix A^N for $\Gamma = 0$ (non-coupled wire). The determinant of the matrix A^N_0 can be obtained analytically; see for example [18]. The above relation, equation (5), can be expressed in terms of Chebyschev polynomials of the second kind, $u_N(x)$, [19]:

$$\det(A^N) = t^N u_N(x) + i\Gamma t^{N-1} u_{N-1}(x) - \frac{\Gamma^2}{4}t^{N-2}u_{N-2}(x), \tag{6}$$

where $x = (E_F - \varepsilon_0)/2t$. Using equations (4) and (6), the transmittance can be written in the general form:

$$T_N = \frac{\Gamma^2 t^2}{[t^2 u_N(x) - \frac{\Gamma^2}{4}u_{N-2}(x)]^2 + t^2\Gamma^2 u^2_{N-1}(x)}. \tag{7}$$

One can obtain a more transparent expression for the transmittance for $|E_F - \varepsilon_0| < 2t$. In this case, we have

$$T_N(E_F, \varepsilon_0, t) = \frac{(\frac{\Gamma}{2})^2(4t^2 - (E_F - \varepsilon_0)^2)}{[(\frac{\Gamma}{2})^2 + t^2]^2 - [(\frac{\Gamma}{2})^2 \cos(N-1)\phi + t^2 \cos(N+1)\phi]^2}, \quad (8)$$

where $\phi = \arccos(x)$ plays the role of the Bloch phase. For $|E_F - \varepsilon_0| > 2t$, the single particle energy ε_0 lies beyond the wire band, and this case is out of our interest. Here the transmittance is expressed only by three parameters of the system: $E_F - \varepsilon_0$, t and Γ.

To find the condition for M-atom conductance oscillations one has to solve the relation $T_k = T_{k+M}$. Using equation (8), the following condition can be obtained:

$$\cos\left(\frac{\pi l}{M}\right) = \frac{E_F - \varepsilon_0}{2t}, \qquad 0 < l < M. \quad (9)$$

This equation indicates the relation between $E_F - \varepsilon_0$ and t which leads to M-atom conductance oscillations of arbitrary length QW. It is worth mentioning that for a period equal to M one has $M - 1$ possible solutions of equation (9).

Most theoretical works have studied the conductance of the quantum wire using *ab initio* calculations; see for example [9, 11, 12, 14]. The analytical solution for the conductance, obtained for any length of the wire, concerns mainly the case of the even–odd conductance oscillations [10, 13]. Using equation (9) one can find that the even–odd oscillations, $T_n = T_{n+M}$, $M = 2$, $n > 0$, are observed only for $E_F - \varepsilon_0 = 0$. In that case the transmittance can be expressed as follows ($k = 0, 1, \ldots$):

$$T_{2k+1} = 1$$
$$T_{2k+2} = \frac{\Gamma^2 t^2}{[t^2 + (\Gamma/2)^2]^2}. \quad (10)$$

For an odd number of atoms in the wire the transmittance is maximal, whereas for an even number the transmittance depends on t, and for large enough t the even-atom transmittance is minimal. For $t = \Gamma/2$ we do not observe even–odd oscillations because the transmittance is maximum, i.e. $T_k = 1$, for all k; see equation (10).

Next, we find analytical formulae for the transmittance in the case of three-atom periodicity, $M = 3$. The relations between $E_F - \varepsilon_0$ and t for three-atom conductance oscillations, obtained from equation (9), are: $E_F - \varepsilon_0 = t$ for $l = 1$ or $E_F - \varepsilon_0 = -t$ for $l = 2$, or equivalently $(E_F - \varepsilon_0)^2 = t^2$. In that case the explicit form of the transmittance of the wire can be written as follows:

$$T_{3k+1} = \frac{\Gamma^2}{t^2 + \Gamma^2}$$
$$T_{3k+2} = \frac{1}{1 + (\frac{\Gamma}{4t})^2} \quad (11)$$
$$T_{3k+3} = \frac{\Gamma^2 t^2}{(t^2 + (\frac{\Gamma}{2})^2)^2}.$$

For $k = 0$ we obtain from the first relation of equation (11) that the transmittance of a single-atom wire, T_1, depends on the coupling strength between QW atoms, t. This is so because here we have $(E_F - \varepsilon_0)^2 = t^2$, and for different values of t the position of ε_0 is also changed (the transmittance of a single-atom wire depends on ε_0).

We find the four-atom periodicity of the transmittance from equation (9) for $M = 4$. The conditions for four-atom oscillations are: $E_F - \varepsilon_0 = \pm\sqrt{2}t$, ($l = 1, 3$) or $\varepsilon_0 = 0$, ($l = 2$). In

the first case we can write the following analytical expressions for the transmittance:

$$
\begin{aligned}
T_{4k+1} &= \frac{\Gamma^2}{2t^2 + \Gamma^2} \\
T_{4k+2} &= \frac{4\Gamma^2 t^2}{(2t^2 + \frac{\Gamma^2}{2})^2 + 4t^2\Gamma^2} \\
T_{4k+3} &= \frac{1}{1 + \frac{\Gamma^2}{8t^2}} \\
T_{4k+4} &= \frac{4\Gamma^2 t^2}{(2t^2 + \frac{\Gamma^2}{2})^2}.
\end{aligned}
\tag{12}
$$

The second case ($E_F - \varepsilon_0 = 0$) corresponds to the even–odd oscillation, which is a special case of every even-atom periodicity.

The general condition for M-atom periodicity, equation (9), and the analytical relations for the transmittance, equations (11), (12), are the first main results of this paper. The explicit analytical equations concern the three- and four-atom periodicities of the transmittance of an arbitrary length wire and are an extension of the two-atom conductance oscillations known so far [6–13].

In a similar way, using equation (9) we can find any atom periodicity in the wire; for example, for $M = 6$ we find $E_F - \varepsilon_0 = \pm\sqrt{3}t$ ($l = 1, 5$), $E_F - \varepsilon_0 = \pm t$ ($l = 2, 4$) or $E_F - \varepsilon_0 = 0$ ($l = 3$) and in these cases we observe six-atom periodicity.

3. Results and discussion

In this section we analyse the details of the periodicity of the conductance and give another general condition for finding the periods of conductance oscillations in the atomic wire. Moreover, the quantum wire charge is discussed.

3.1. M-atom oscillations

The transmittance of the QW coupled to the leads, in the general case, is expressed by equation (8). For special cases one can use the explicit analytical equations for the transmittance, equations (10)–(12) which describe two-, three- and four-atom periods and are valid for arbitrary length wire. In our calculations we set $E_F = 0$ and all energies are expressed in units of Γ. The conductance is in units of $2e^2/h$.

In figure 1, we show the conductance as a function of the energy ε_0 and the length of the wire ($N = 1, \ldots, 15$). The coupling strengths between atoms are $t = 2$ (the upper panel) and $t = 4$ (the lower panel). White represents the maximum value of the conductance ($G = 1$) whilst black corresponds to $G = 0$. The main conclusions concerning figure 1 are as follows:

(1) For an N-atom wire we observe N maxima of the conductance (and the transmittance); for example, for a three-atom wire, $N = 3$, there are three white fields. It is known that a finite periodic system consisting of N cells exhibits a pattern of N narrow resonances in each band; see for example [20]. Moreover, it can be seen that the conductance possesses nonzero values only in the regime of $|\varepsilon_0| < 2t$; this is better shown for $t = 2$ (the upper panel of figure 1).

(2) For a larger value of t ($t = 4$, the lower panel), the peaks of the conductance are separated and are more visible than for $t = 2$ (the upper panel). In the weak coupling regime ($t = 2$) the distances between the nearest conductance peaks are shorter and the values of the conductance (between these peaks) are not equal to zero: we observe a grey (blue)
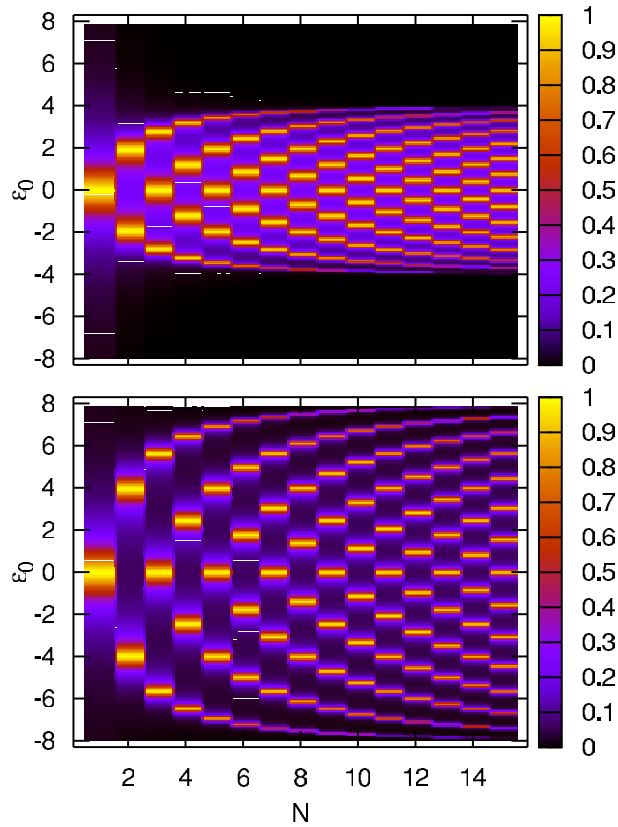
Figure 1. The linear conductance as a function of the wire's length, N, and electron energy ε_0 for $t = 2$ (upper panel), and $t = 4$ (lower panel). The black (light) colour corresponds to $G = 0$ ($G = 1$); $\Gamma = 1$.

(This figure is in colour only in the electronic version)

colour instead of black. For $N = 1$ we observe the same structure of the conductance, independent of t, as in that case we have a single-atom wire.

(3) We observe the even–odd conductance oscillations for $\varepsilon_0 = 0$, and these oscillations are easily visible in figure 1 as alternately white and black colours. We find the three-atom period of the conductance for $\varepsilon_0 = \pm t$ and in our case for $t = 4$ (figure 1, the lower panel); we observe this for $\varepsilon_0 = \pm 4$. The four-atom period of the conductance is visible for $\varepsilon_0 = \pm\sqrt{2}t \simeq \pm 5.65$, etc. One can easily find the M-atom conductance periodicity of the wire in the following way. For an N-atom wire we obtain the maximum values of the transmittance versus the energy ε_0 and for these values of ε_0, an $M = (N + 1)$ period of the conductance appears. For example, for $t = 4$ and $N = 2$ (5), the maximum values of the conductance are for $\varepsilon_0 = \pm 4$ ($\varepsilon_0 = 0, \pm 4, \pm 4\sqrt{3}$), and in these cases we find $M = N + 1 = 3$ (6) periodicity. Of course the second case (six-atom period) is degenerated as it also includes the two- and three-atom periods (for $\varepsilon_0 = 0$ and for $\varepsilon_0 = \pm t$). Moreover, the maxima of the transmittance can be found from the retarded Green function by solving the following equation: $\operatorname{Re} G^{\mathrm{r}}_{1N} = 0$. This conclusion is valid for the condition $t > \Gamma/2$, which is satisfied in our case. For very weak couplings t, M-atom periodicity should be found from the general equation (9).
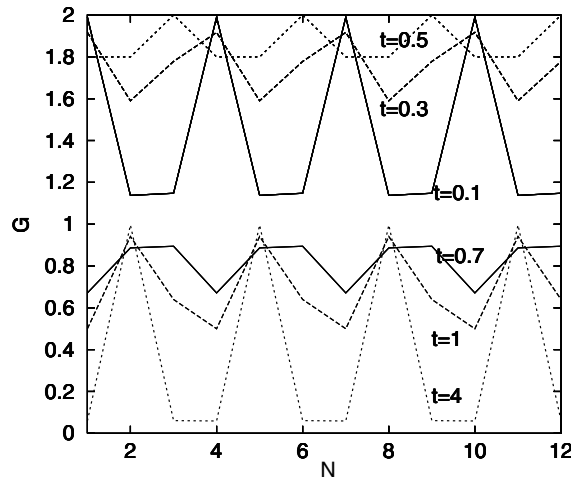
Figure 2. The conductance versus the length of the wire N for $\varepsilon_0 = t = 0.1, 0.3, 0.5$ (the upper curves) 0.7, 1, 4 (the lower curves). The lines are plotted for better visualization.

To conclude, M-atom conductance oscillations appear for $\varepsilon_0 = E_{\max}$ (for $t > \Gamma/2$) where $E_{\max}$ is the energy where the transmittance of $N = (M-1)$-atom wire possesses the maximum value. The above conclusion is the second main result of this paper.

3.2. The special case: $M = 3$

As was shown in the previous section, the three-atom period of the conductance is observed for $E_{\mathrm{F}} - \varepsilon_0 = \pm t$, and in this case the transmittance of an N-atom wire can be expressed by equation (11). In figure 2 we show the conductance versus the length of the wire for $\varepsilon_0 = t = 0.1, 0.3, 0.5, 0.7, 1$ and 4 (from very weak to strong coupling strength). The lines are separated into upper and lower parts and are plotted for better visualization. The most interesting conclusions concerning the three-atom periodicity of the conductance are as follows.

(1) The conductance of every $(3k + 1)$th atom $(k = 0, 1, \ldots)$ gets smaller and smaller as the coupling t increases. This results from the equation for the transmittance, equation (11) for $(3k + 1)$, where t appears only in the denominator. In the same way we can analyse the other cases. For $(3k + 2)$th atom the conductance increases with increasing t and for $(3k + 3)$th atom the conductance varies depending on the value of t.

(2) We observe the maximum value of the conductance for (a) $(3k + 1)$th-atom in the case of $t < \Gamma/2$, cf the curve for $t = 0.1$; (b) $(3k + 2)$th-atom in the case of $t > \Gamma/2$, cf the curve for $t = 4$; (c) $(3k + 3)$th-atom in the case of $t = \Gamma/2$, cf the curve for $t = 0.5$. This is a very interesting result because from the position of the maximum value of the conductance one can draw conclusions about the coupling strength between atoms, t.

(3) Using equation (11) we can find that for $t \in (\Gamma/2; \Gamma/\sqrt{2})$ the conductance satisfies the following 'lesser' relation: $G_{3k+1} < G_{3k+2} < G_{3k+3}$ and for $t = \Gamma/2(t = \Gamma/\sqrt{2})$ we have $G_{3k+1} = G_{3k+2} < G_{3k+3}$, $(G_{3k+1} < G_{3k+2} = G_{3k+3})$, cf the curve for $t = 0.5$ $(t = 0.7)$. However, it is impossible to get the 'greater' relation for the conductance, $G_{3k+1} > G_{3k+2} > G_{3k+3}$.

In the same way, using equation (12), we can describe the four-atom period of the conductance. It is interesting that for any t we never get $G_{4k+1} < G_{4k+2} < G_{4k+3} < G_{4k+4}$ or $G_{4k+1} > G_{4k+2} > G_{4k+3} > G_{4k+4}$. So the 'greater' and the 'lesser' relations for the conductance cannot be satisfied in this case.

Analysing the results presented in figures 1, 2 and relations (11), (12) one can conclude that in the case of M-atom periodicity, we observe the maximum value of the conductance for every $N = [M(k + 1) - 1]$ atom; for example, for $M = 3$ the conductance is maximum for $N = 2, 5, 8, \ldots$; cf the broken line in figure 2, the lower curves. This can be explained in terms of the transmittance, equation (11), where for $t \gg \Gamma/2$ we have $T_{3k+1} = 0$, $T_{3k+2} = 1$, $T_{3k+3} = 0$. In the general case one can obtain from equation (8) that the transmittance $T_{M(k+1)-1} \equiv 1$ for the condition given by equation (9) and $t \gg \Gamma/2$. This conclusion is the third main result of the paper.

3.3. QW charge

In this subsection we analyse the local and averaged charges localized in the QW. We can obtain the charge at site i from the following relation: $Q_i = \frac{-1}{\pi} \int_{-\infty}^{E_F} \operatorname{Im} G_{ii}^r(E) \, dE$. In figure 3 we show the average QW charge $\langle Q \rangle$, $\langle Q \rangle = \frac{\sum_i^N Q_i}{N}$, as a function of the wire's length, N, for $t = 4$ and for (a) $\varepsilon_0 = 0$ (dotted line); (b) $\varepsilon_0 = -t, +t$ (upper and lower broken lines); (c) $\varepsilon_0 = \sqrt{2}t$ (solid line); (d) $\varepsilon_0 = \sqrt{3}t$ (thick line). The positions of ε_0 we consider here correspond to the two-, three-, four- and six-atom oscillations of the conductance. Additionally, the crosses in figure 3 represent the local charge Q_i at site i for $\varepsilon_0 = -t$, i.e. the upper broken line is obtained by averaging the charges Q_i for every N. For $N = 1$ we have only one cross; for $N = 2$ there are two crosses but in that case $Q_1 = Q_2$. In the case of $N = 3$, $Q_1 = Q_3 \neq Q_2$ and only two crosses are visible, and so on. One can see that the values of the local QW charges Q_i are rather close to their average value. Except for the two-atom oscillation the average QW charge, $\langle Q \rangle$, oscillates with a period depending on the conductance oscillation period. The average charge of the wire tends to a constant value as the length of the wire increases. This effect is visible for cases (b)–(d) (the broken, thin and thick lines). We conclude that the average charge of the wire is linked with the period of the conductance oscillations. Here we analyse this effect in detail. The average charge of the wire for the even–odd oscillations (two-atom period), $\varepsilon_0 = 0$, is $1/2$, and it does not depend on N (the dotted line). For the three-atom period we find, for large N, that the average QW charge is equal to $1/3$ for $\varepsilon_0 = +t$ (the lower broken line) and $2/3$ for $\varepsilon_0 = -t$ (the upper broken line). For the four-atom period the average QW charges are $1/4$ for $\varepsilon_0 = +\sqrt{2}t$ (the thin line); $3/4$ for $\varepsilon_0 = -\sqrt{2}t$ (not shown in figure 3) and $1/2$ for $\varepsilon_0 = 0$ (the special case of the two-atom period). These results are in agreement with those of [14] where the filling of the QW results in the periodicity of the conductance. According to this work, the periods of the conductance oscillations are determined by the inverse of the conductance band filling. However, in our case we have found that there are few characteristic fillings of the wire which indicate the periodicity of the conductance, for example for the three-atom period: $\langle Q \rangle = 1/3$ or $2/3$. This results directly from equation (9) where for an M-atom period we have $M - 1$ possible solutions of this equation.

In general, for M-atom periodicity, the average charge of the wire can take $(M-1)$ possible values: $1/M, 2/M, \ldots, (M - 1)/M$; here we consider also the degenerate fillings, e.g. $2/4$, $2/6$, etc. This effect means that the QW charge determines the period of the conductance oscillations unambiguously, whereas knowledge of the period does not allow us to indicate the QW charge exactly. This general conclusion is the fourth main result of the paper.
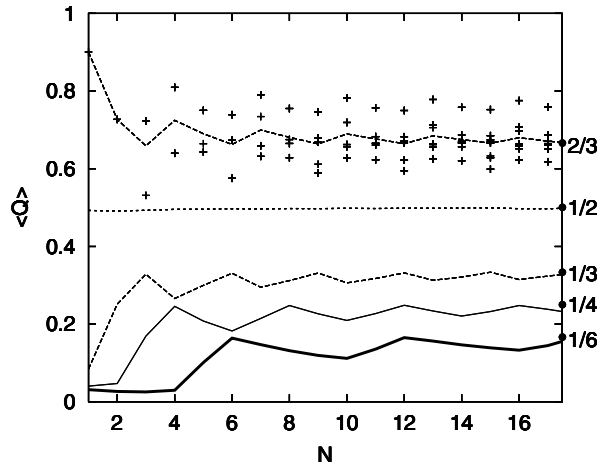
Figure 3. The average QW charge versus the length of the wire N for $t = 4$ and $\varepsilon_0 = 0$—dotted line, $\varepsilon_0 = -4$, (+4)—the upper (lower) broken line, $\varepsilon_0 = -4\sqrt{2}$—thin line, $\varepsilon_0 = -4\sqrt{3}$—thick line. The crosses correspond to the local charge of the i-atom for $\varepsilon_0 = -4$. The right-hand side numbers represent fillings of the long-length wires.

4. Conclusions

In summary, the transmittance and the conductance of a finite atomic wire have been calculated using the Green function method and a tight-binding Hamiltonian. For the symmetric case, assuming the same electron energies of all atoms in the wire and the same coupling strengths between them, one can write the main and new results of this paper as follows.

(1) Analytical solutions for the transmittance have been obtained for any length of wire, equations (7), (8), and also equations (11), (12) which describe the three- and four-atom periods of the conductance oscillations.

(2) The general conditions on any M-atom periodicity of the conductance have been obtained, equation (9), and discussed. One can also find the condition for $(N + 1)$-periodicity from the maximum values of the transmittance versus the energy of an N-atom wire.

(3) Some interesting results of $M > 2$-atom periodicity have been discussed. The main and general result concerns the maximum value of the conductance. In the case of M-atom periodicity we observe the maximum value of the conductance for every $N = [M(k+1)-1]$ atom, $k = 0, 1, \ldots$.

(4) For M-atom periodicity, the average charge of the wire can take $(M - 1)$ possible values: $1/M, 2/M, \ldots, (M - 1)/M$, and in this case there are $(M - 1)$ possible fillings $\langle Q \rangle$ (degenerate and non-degenerate) of the wire.

There are four main results of this paper. These results and also others included in the paper can be very useful for future experiments, i.e. by analysing the structure of the conductance versus the length of the wire one can draw conclusions about the coupling strength between QW atoms, or from the distance of the maximal values of the conductance about the periodicity. Of course in an experiment one needs to measure the conductance for infinitesimal bias across the wire, for the Fermi energy of the leads. If $E_F = \varepsilon_0$ only the even–odd oscillation can be investigated, so one needs to change the energy ε_0 or the coupling t to measure the other oscillations, $M > 2$. To prepare a such experiment one can use for example metallic wires on vicinal surfaces [1, 2]. One end of the wire can be coupled with a special electrode (prepared

for example by an epitaxy method) and the second could be the STM tip. The current can flow from the electrode to the tip through the atoms which are between them. By changing the position of the STM tip we can change the number of atoms between the electrode and the tip (the length of the wire). In such a wire one can change the position of ε_0 by applying the potential to the vicinal surface: the coupling t remains unchanged. It is only one experimental possibility to measure the conductance oscillations of the wire and it is believed that the results presented in this work will be confirmed experimentally in the near future.

Acknowledgments

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