Electron transport through a strongly correlated monoatomic chain

M. Krawiec * and T. Kwapiński
Institute of Physics and Nanotechnology Center, M. Curie-Skłodowska University,
pl. M. Curie Skłodowskiej 1, 20-031 Lublin, POLAND

Abstract

We study transport properties of a strongly correlated monoatomic chain coupled to metallic leads. Our system is described by tight binding Hubbard-like model in the limit of strong on-site electron-electron interactions in the wire. The equation of motion technique in the slave boson representation has been applied to obtain analytical and numerical results. Calculated linear conductance of the system shows oscillatory behavior as a function of the wire length. We have also found similar oscillations of the electron charge in the system. Moreover our results show spontaneous spin polarization in the wire. Finally, we compare our results with those for non-interacting chain and discuss their modifications due to the Coulomb interactions in the system.

Key words: quantum wire, conductance oscillations, electron correlations
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1. Introduction

Recently one-dimensional (1D) quantum wires (QW) have attracted much attention due to their potential applications in nanoelectronics [1] and quantum computing [2]. The knowledge of the transport properties of such structures is crucial for the design and fabrication of the nanodevices. On the other hand the quantum wires, although conceptually simple, are very interesting from scientific point of view as they display extremely rich phenomena, very often different from those in two and three dimensions [3,4]. The understanding of the properties of such 1D objects is a major challenge in the field of nanophysics.

The conductance of the quantum wires has been studied both experimentally and theoretically by number of authors (see [5] for a review). The experimental studies require advanced techniques of fabrication of such structures. Those include: growing of QW on metallic surfaces [6,7], scanning tunneling microscope techniques [8] or mechanically controlled break junctions [5,9,10]. Those fabrication techniques allowed for revealing of many phenomena like charge quantization in units of $G_0 = 2e^2/h$ [11], deviations from that (0.7(2e^2/h) anomaly) [12], spin-charge separation (Luttinger liquid) [13], oscillations of the conductance as a function of the length of the chain [9,10] or spontaneous spin polarization in QW [12,14].

The purpose of the present paper is two fold.
The first one is to investigate the oscillations of the conductance as a function of the wire length in the case of strong Coulomb interactions. The oscillatory behavior of the conductance manifests itself as a maximum of the conductance when a number of the atoms in a wire is odd and minimum when the number is even. This effect is known as the even-odd conductance oscillations. Most common examples are the oscillations with a period of two [9, 10, 15, 16, 17, 18] and four atoms [19]. However, those analytical formulas remain valid for noninteracting wire only. In the presence of strong Coulomb interactions the even-odd oscillations with a period of two atoms have been also found [21, 22, 23, 24, 25, 26]. The mean period is two atoms coupled to the left L and right R lead described by the following Hamiltonian in the limit of strong on-site Coulomb interaction (\(U_i \to \infty\)) in the slave boson representation where the real wire electron \(d_{i\sigma}\) is replaced by the product of the boson \(b_i\) and the fermion \(f_{i\sigma}\) operators (\(d_{i\sigma} = b_i^\dagger f_{i\sigma}\)) [29, 30, 31]:

\[
H = \sum_{\lambda k \sigma} \varepsilon_{\lambda k} c_{\lambda k \sigma}^\dagger c_{\lambda k \sigma} + \sum_{i\sigma} \varepsilon_i f_{i\sigma}^\dagger f_{i\sigma} + \sum_{(ij), \sigma} t_{ij} f_{i\sigma}^\dagger b_j^\dagger f_{j\sigma} + \sum_{k \in L(R),\sigma} V_{L(R)k} c_{L(R)k \sigma}^\dagger b_{1(N)\sigma}^\dagger f_{1(N)\sigma} + \text{h.c.},
\]

where \(c_{\lambda k \sigma}\) stands for the electron with the single particle energy \(\varepsilon_{\lambda k}\), the wave vector \(k\) and the spin \(\sigma\) in the lead \(\lambda = L, R\). \(\varepsilon_i\) denotes the wire energy level at site \(i\), \(t_{ij}\) is the hopping integral of the electrons between neighboring wire sites \(i\) and \(j\), and \(V_{L(R)k}\) is the hybridization matrix element between electrons at site \(1(N)\) and those in the lead \(L(R)\).

In the linear response and at the zero temperature the conductance \(G\) is proportional to the total transmittance \(T\), i.e. \(G = 2e^2/h T\). In our case the transmittance is given by [20, 32]:

\[
T_N(E) = \sum_{\sigma} \Gamma_L \Gamma_R |G_{1 N\sigma}^r(E)|^2,
\]

where \(G_{1 N\sigma}^r\) is the retarded Green function (GF) connecting the ends of the wire (sites \(1\) and \(N\)) and \(\Gamma_L(R) = 2\pi \sum_{k} |V_{L(R)k}|^2 \delta(E - \varepsilon_{L(R)k})\). In calculations we have assumed constant bare density of states in the leads.

Using the equation of motion technique for the retarded GF with Hamiltonian (1) one can write the general matrix equation for \(G_{ij\sigma}^r\) in the form:

\[
\hat{A}_{ij} G_{ij\sigma}^r = \hat{N}_{ij\sigma}.
\]

Due to the strong on site Coulomb interactions in the wire \(U_i\), which is assumed to be infinity in our case, the problem cannot be solved exactly and one has to make approximations of the higher order GFs emerging in the equation of motion for the retarded GF \(G_{ij\sigma}^r = \langle \langle b_i^\dagger f_{i\sigma}^\dagger | f_{j\sigma}^\dagger b_j \rangle \rangle_E\). We have used Hubbard I like approximation [31] according to which the GF \(\langle \langle f_{i\sigma}^\dagger f_{j\sigma} | f_{i\sigma}^\dagger f_{j\sigma} \rangle \rangle_E\) is approximated by \(\langle f_{i\sigma}^\dagger f_{j\sigma} \rangle \langle b_i^\dagger f_{i\sigma}^\dagger f_{j\sigma} b_j \rangle_E\) and the other higher order GFs are neglected. This approximation is reasonably good for not very large
values of the hopping \( t \) and neglects higher order processes, like for example the Kondo effect.

Within the present approximation scheme \( \hat{A}_\sigma \) in the Eq. (3) is \( N \times N \) tridiagonal symmetric matrix with the elements:

\[
\hat{A}_\sigma = \begin{pmatrix}
(E - \varepsilon_i)\delta_{i,j} + i\Gamma/2(\delta_{i,1}\delta_{j,1} + \delta_{i,N}\delta_{j,N}) -
t[(1 - n_{i-\sigma})\delta_{i,i+1} + (1 - n_{i+1-\sigma})\delta_{i+1,i}]
\end{pmatrix}
\]

and \( \hat{N}_\sigma \) is the diagonal matrix of the form:

\[
\hat{N}_\sigma = (1 - n_{i-\sigma})\delta_{i,j},
\]

with \( n_{i\sigma} = \langle f_{i\sigma}^+ f_{i\sigma} \rangle = -\frac{i}{\pi} \int dE ImG_{i\sigma}(E) \) being the average occupation of the electrons with spin \( \sigma \) at site \( i \).

3. Results

In numerical calculations we have assumed all the wire site energies to be equal (\( \varepsilon_i = \varepsilon_0 \)) and similarly hopping integrals \( t_{ij} = t \). All energies are measured with respect to the leads Fermi energy \( E_F = 0 \) in units of \( \Gamma = \Gamma_L = \Gamma_R = 1 \). Moreover, the occupation \( n_{i\sigma} \) is calculated self-consistently on each wire site.

To find the condition for M-atom conductance oscillations one has to solve the relation: \( T_N = T_{N+M} \), where \( T_N \) \((T_{N+M})\) is the transmittance of the wire consisted of \( N \) \((N + M)\) atoms, given by Eq. (2). In general, for \( U_i \to \infty \) it is not possible to get analytical expression for the oscillations condition without further assumptions. Note that for \( U_i = 0 \) the problem can be solved exactly and such condition can be found [20]. In this case it reads

\[
\cos\left(\frac{\pi l}{M}\right) = \frac{E_F - \varepsilon_0}{2t(1 - n_{i\sigma})},
\]

with \( l = 1, 2, ... M - 1 \). Unfortunately, one has to know the average occupation \( n_{i\sigma} \). The only case of \( M = 2 \) can be solved analytically. As one can see from Eq. (6) the period of two can be obtained for \( E_F - \varepsilon_0 = 0 \), i.e. when the wire single particle energy levels all coincide with the Fermi energy.

In Fig. 1 the total linear conductance \( G = \sum_{\sigma} G_{\sigma} \) is plotted as a function of the wire length \( N \) and the energy level \( \varepsilon_0 \) for \( t = 4 \). As one can see all the figures show similar patterns with the regions of large and small conductances. Moreover, for \( \varepsilon_0 = 0 \) behavior of the conductance is the same in all three cases which leads to the conclusion that correlations are not important in this case. It always shows even-odd \((M = 2)\) oscillations. Away from \( \varepsilon_0 = 0 \) correlations strongly modify the conductance, shifting the maxima of \( G \) (for fixed \( N \)) towards lower (higher) energies for \( \varepsilon_0 > 0 \) \((\varepsilon_0 < 0)\). This is due to the modification of the wire hopping, which depends now on the occupation \( n_{i\sigma} \) (see Eq. (4)). This effect also leads to the strong asymmetry for positive and negative energies. For negative (positive) wire energies the occupation is large (small), therefore effective hopping \( t = t(1 - n_{i-\sigma}) \) is small (large), thus the conductance decreases (increases). Note that there is no such asymmetry in the case of \( U_i = 0 \). Moreover, different periods of the conductance oscillations can be observed, depending on the position of the wire energy level.

Another important finding is that the wire shows spontaneous spin polarization. It is well known that in strictly 1D wire the spin polarization is prohibited due to the Lieb-Mattis theorem [28]. However this theorem is valid for infinite wire only. In experimental situation the wire is always connected to the electrodes and this is why the spin polarization is observed experimentally [12,14]. Interestingly, it was predicted recently that even infinite wire, but of the zig-zag shape, can also exhibit the spin polarization [33].

The total conductance in ferromagnetic case is shown in the bottom panel of Fig. 1. Again, unlike for \( U_i = 0 \), the conductance pattern shows strong asymmetry for positive and negative energies. Note that for negative energies there are no differences between \( G_{\text{ferro}} \) (bottom panel) and \( G_{\text{para}} \) (middle panel). For such energies iterations always con-
Fig. 1. The total linear conductance $G = \sum_{\sigma} G_{\sigma}$ as a function of the wire length $N$ and the wire energy level $\varepsilon_0$ for $U_i = 0$ (top panel), $U_i \to \infty$ in paramagnetic configuration $n_{i\sigma} = n_{i\bar{\sigma}}$ (middle panel) and ferromagnetic one (bottom panel).

Fig. 2. The difference between spin up and spin down conductance as a function of the wire length $N$ and the wire energy level $\varepsilon_0$.

The total linear conductance $G = \sum_{\sigma} G_{\sigma}$ as a function of the wire length $N$ and the wire energy level $\varepsilon_0$ for $U_i = 0$ (top panel), $U_i \to \infty$ in paramagnetic configuration $n_{i\sigma} = n_{i\bar{\sigma}}$ (middle panel) and ferromagnetic one (bottom panel).

verge to paramagnetic solution. This can be again explained by effect of the hopping modification. For negative energies the wire occupation is large, thus the effective hopping $t = t(1-n_{i\sigma} \bar{\sigma})$ is small. One can imagine in this case that the electrons are more localized and it is more convenient for them to spend more time on the same site than move to another one. Moreover in the case of the lack of the inter-site interactions any collective phenomenon is not possible. Situation is different for positive energies. In this case the electrons are more mobile, as the effective hopping is larger due to the small values of the wire occupations. Thus they interact with each other via hopping and it is possible and energetically more favorable to get the ferromagnetic state. The hopping, which is the correction to the position of the wire energy levels, leads to the effective splitting of this levels. Thus the conductance is spin polarized in this case. It can be read off from Fig. 2, where the difference between spin up and spin down conductance is displayed. It turns

out that the strongest differences between $G_{\uparrow}$ and $G_{\downarrow}$ can be found for intermediate values of $\varepsilon_0$. For energies close to $E_F$ the modifications are weak due to the small values of the hopping while for higher energies the wire occupation is very small thus the difference between spin dependent effective hopping can be neglected. Finally it is worthwhile to note that for $N = 1$ (single atom) there is no ferromagnetic solution as the ferromagnetism is governed by inter-site hopping in our case. Whether this spontaneous spin polarization is a true effect or a drawback of the approximation used remains an open question, as it is known that the mean
field like theories overestimate the role of the magnetism. The problem will be further studied.

Corresponding spin polarization $n^\uparrow - n^\downarrow$ ($n_{\sigma} = \sum_i n_{i\sigma}/N$) is shown in Fig. 3. As one can see the spin polarization pattern is similar to that of the conductance differences (see Fig. 2). In Fig. 4 we show the conductance (left panels) and the occupation (right panels) as a function of the wire length for a number of the energy levels $\varepsilon_0$ in the paramagnetic configuration. The values of $\varepsilon_0$ have been chosen in such a way that they lead to the maxima of the conductance for $N = 1, 2$ and 3 atom wire. For example, the maxima of the conductance of the $N = 2$ atom wire correspond to $\varepsilon_0 = -2.298$ and 3.135 (see the middle panel of Fig. 1). These maxima in $U_i = 0$ case give the periods of the conductance oscillations. To find $M$-atom period it is enough to determine the maxima of the conductance for $N = M - 1$ atom wire [20]. As one can read off from Fig. 4, depending on $\varepsilon_0$, one gets different periods of the conductance oscillations. Moreover, except for the special case of $M = 2$, the amplitude of the oscillations decreases with the wire length. This is a kind of damped oscillations. No such effect has been observed for $U_i = 0$ [20].

At this point we would like to comment on the other results known in the literature. The even-odd ($M = 2$) oscillations problem was extensively studied within the second order perturbation theory in $U_i$ (SOPT) [21,22] and the numerical renormalization group (NRG) approach [23,24]. The results show similar behavior of the conductance for odd number of atoms in a wire: it always reaches the unitary limit ($\frac{2e^2}{h}$), independently of $U_i$. Such behavior is a consequence of the Kondo effect. However, in our case the situation is slightly different, as we get $M = 2$ oscillations in the mixed valence regime only ($\varepsilon_0 = 0$), where the Kondo effect is excluded. Thus our even-odd oscillations are caused by the resonances associated with the energy level structure of the chain rather than the Kondo effect. On the other hand, the conductance for even number of atoms in a wire is strongly suppressed, in agreement with SOPT [21,22] and NRG approaches [23,24]. However, NRG calculations show that the conductance exponentially depends on $U_i$, and in the limit of $U_i \to \infty$ vanishes, contrary to our results, as we get non-zero values of $G$ (see Fig. 4), depending on the hopping $t$. The conductance vanishes in the limit of very large or very small values of $t$. Interestingly, when $t = \Gamma/2$, the conductance reaches the unitary limit and shows no oscillations, i.e. is equal to $\frac{2e^2}{h}$ for even and odd $N$.

Figure 4 (right panels) shows the wire length dependent occupation which also oscillates with the

![Fig. 3](image)

**Fig. 3.** The spin polarization as a function of the wire length $N$ and the wire energy level $\varepsilon_0$.

![Fig. 4](image)

**Fig. 4.** The total conductance (left panels) and the occupation (right panels) vs. wire length. The left panels show the conductance with different oscillations periods (2 to 4) from top to bottom. The positions of the wire energy levels are indicated in the figure.
same period as the conductance does, except for the special case of $\varepsilon_0 = 0$ ($M = 2$), where the occupation remains constant. Moreover, the Coulomb interactions $U_i$ lead to the reduction of the occupation oscillation amplitude. Similar effect, albeit for small $U_i$, has been found within self-consistent Hartree-Fock approximation [34].

In ferromagnetic case the situation is more complex. For positive values of $\varepsilon_0$ due to the splitting of the conductance maxima (see Fig. 1) no regular oscillations have been observed. On the other hand, for $\varepsilon_0 < 0$ one gets such oscillations but in this case the solutions remain always paramagnetic. Figure 5 shows the comparison of the conductance and the occupations in paramagnetic and ferromagnetic configurations for the wire consisted of five atoms. For negative energies, as discussed before, there are paramagnetic solutions only. For $N > 1$ and $\varepsilon_0 > 0$ the ferromagnetic solutions emerge in certain energy regimes. In this case $n_{\uparrow} \neq n_{\downarrow}$ and resulting conductance peaks are split. Interestingly, the spin polarizations occurs only in the regimes where the occupation has a large slope or the total conductance has a maximum. Moreover, the splitting of the conductance leads to the fact that $G_{\text{ferro}}$ shows more maxima than $G_{\text{para}}$. A number of maxima of $G_{\text{ferro}}$ is related to the wire length (number of atoms - $N$) and for odd $N$ it gives $(3N - 1)/2$ maxima, while for even $N$ one observes $3N/2$ maxima. In paramagnetic case it is always equal to a number of atoms $N$ in the wire (compare top panels of Fig. 5).

Finally we would like to comment on the validity of our approach. The present calculations completely neglect the Kondo effect which is important at low temperatures and $\varepsilon_d < 0$. We expect some modifications in this regime, as this effect leads to the corrections of the conductance of the order of $e^2/\hbar$. Thus our results apply for temperatures higher than the Kondo temperature. On the other hand, we do not expect any qualitative modifications in the mixed valence and the empty regimes ($\varepsilon_d \geq 0$).

4. Conclusions

In summary we have studied the conductance oscillations of the strongly interacting wire as a function of the wire length. We have found that strong Coulomb interactions significantly modify the periods of the oscillations showing strong asymmetry for negative and positive wire energy levels. They also lead to the suppression of the conductance with increasing wire length. There are no such effects for noninteracting wire. Moreover, strong interactions lead to the spontaneous spin polarization for positive wire energies, observed in experiments.

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