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Effects of Coulomb interactions in electron transport through short molecular chains

TOMASZ KOSTYRKO[1*], BOGDAN R. BUŁKA[2]

[1]Institute of Physics, A. Mickiewicz University, Umultowska 85, 61-614 Poznań, Poland

[2]Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17, Poznań, Poland

Charge transport properties of short molecular chains connected to electrodes are studied using the non-equilibrium Green function method. The chains are described using a single-orbital Hubbard model. In the weak interaction range and low-temperature limit, the current flowing through the system was analysed within the Hartree–Fock approximation (HFA). It was found that for a weak coupling between the molecule and the leads *I–V* characteristics can be represented as a sequence of plateaus, alternating with regions of a finite slope. This finite slope in the *I–V* characteristics is related to the self-consistent molecular level being pinned down to the Fermi levels of the electrodes over a finite voltage regions. It is also related to a continuous change in the charge state of the molecule. In the strong repulsion limit, the HFA method is no longer credible and we resort to decoupling the equations of motion (EOM) for the Green functions of the chains, in order to treat all intrachain correlations and hopping exactly but to neglect some correlations between the molecule and the leads. A comparison of the results obtained with these two approaches for the same parameters allows us to make general observations concerning the role of correlations in transport through molecular junctions.

Key words: *charge transport through molecule; electron–electron interactions*

1. Introduction

Fast development of nanotechnology has led to manufacturing molecular junctions which are expected to replace silicon-based devices in electronic applications in a near future [1]. Several experimental methods are currently being used to obtain junctions with nanometer-sized molecules trapped between their macroscopic metallic leads. Despite technical differences between various experimental methods, the accumulated data show some general features of molecular junctions that involve short atomic and molecular wires.

[*]Corresponding author, e-mail: Akos@hts1.physd.amu.edu.pl.

Monatomic chains, for instance gold atoms pulled out from gold leads by a STM tip [2–4] or an H_2 molecule trapped between platinum electrodes [5], behave like perfect ballistic conductors at small voltages, with the conductance hardly depending on chain length. All the damping and Joule heating takes place in the electrodes up to the voltage threshold (of the order of several dozens of millivolts), when the onset of inelastic scattering due to electron coupling with intrachain vibrations starts to reduce the current in a step-wise fashion by several percent. For atoms with partially filled s-levels, the zero-voltage conductance is close to the quantum unit, $G_0 = 2e^2/h$, and the current can be as large as 80 μA (for a voltage of about 1 V). This indicates that a strong coupling exists between the electrodes and atomic chains, as well as that there is a single channel for transmission.

Junctions involving short organic wires, like benzene dithiolate, [6], bithiolterthiophene [7], alkane dithiolates [8], or 4,4-bipyridinium [8] usually support relatively low currents, rarely exceeding 1 μA. The resistance of polymeric wires usually grows exponentially with their length [8]. A much smaller conductance of junctions with organic wires as compared to ones with s-orbital atomic wires is due to, first of all, a rather small overlap of the s-orbital of the metallic leads and p-orbitals of the HOMO-LUMO subsystem of the molecules. Also, a Schottky-like barrier created at the bonding atom of the molecule (often sulphur, nitrogen, or carbon) can be responsible for this weak coupling. Despite weak coupling to the leads, this coupling significantly perturbs the molecular levels and the differential conductance exhibits relatively wide peaks with halfwidths of the order of 1 V, even at temperatures much smaller than estimated for the coupling and separations of the levels.

Theoretical works aiming to describe transport characteristics in molecular junctions range from simple parametric models using tight binding models, [9–11] through extended Hückel calculations [7, 12–15], to *ab initio* methods [16–21] using density functional theory (DFT). While these methods differ in the number of atomic orbitals of the molecules included in computations and the way of treating the electron –electron interactions, they all belong to the class of single-particle approaches and neglect the effects of electron correlation. On the quantitative level, first principles computations often overestimate the current transmitted through junctions with organic molecules by more than an order of magnitude [18, 21], even if the shape of the *I–V* curves is fairly well reproduced. Parametric (semiempirical) calculations can be used to fit experimental values of current for a given voltage by a proper choice of the coupling parameter (or a function) Γ but in this case the overall shape of the current –voltage (*I–V*) curve is not described well [13, 7]. The value of Γ, taken in order to reproduce the values of the current, usually gives too narrow peaks in the corresponding differential conductance curves or too sharp steps in the *I–V* curve.

In the face of a quantitative disagreement between results for single particle computations and experimental findings, it is natural to ask about the role of the hitherto neglected effects of electron correlation in a more complete understanding of the transport properties of molecular junctions including organic molecules. As we know

from work performed on systems of lithographically defined artificial atoms, i.e. quantum dots (QD), the effects of electron correlation can be very important, and manifest themselves in the Coulomb blockade [22] or Kondo effect [23]. Although correlation driven phenomena in QDs are observed at very low temperatures (1 K or less), the corresponding effects in molecular junctions could play a role in a higher temperature range as a result of much higher (by a factor of 10^3) energy parameters, i.e. intradot Coulomb repulsion, coupling to the leads, coupling between neighbouring QDs, etc.

The purpose of the present work is to provide some examples of computations, supported by parametric models, for a very simple system (2-atom molecule), using both a quasiparticle approach and a method that treats electron correlations within the molecule in an exact manner. A comparison of the two approaches, within the same parameter range, may elucidate the role of electron correlation in transport through molecular junctions. Although such a comparison is possible only for systems with a very small number of electron degrees of freedom (atomic orbitals), an extension of the present work to larger systems could reveal some generalizations of the observed tendencies.

2. Quasiparticle description of electron transport

We describe the system of a molecule connected to macroscopic leads by the following Hamiltonian

$$H = \sum_{\alpha=L,R} H_\alpha + H_T + H_M \tag{1}$$

where H_α is the one-particle Hamiltonian of the left (for $\alpha = L$) or right (for $\alpha = R$) lead, H_T describes one-particle tunneling between the leads and the molecule (for simplicity, we assume that the molecule is attached to the leads by means of a single atom), and H_M is the Hamiltonian of the molecule.

The molecular part of the system is described by a single-orbital Hubbard Hamiltonian:

$$H_M = \sum_{jm\sigma} t_{jm} d^+_{j\sigma} d_{m\sigma} + \sum_{j\sigma} E_j n_{j\sigma} + U \sum_j n_{j\sigma} n_{j-\sigma} \tag{2}$$

where t_{jm} is the intramolecular hopping parameter, U is the on-site electron repulsion, and the site energy E_j includes a contribution from the bare external potential generated by a voltage applied to the leads (the potential ramp [15]).

In order to analyse the transport characteristics of such a molecular junction, we use the non-equilibrium Green function method*. The current is computed using a general formula obtained by Meir and Wingreen [25]

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*For the technique of the non-equilibrium Green functions and its applications in electronic transport, see Ref. [24].

$$J = \frac{ie}{h}\int d\omega \Gamma_L \left[f_L (G^r_{LL\sigma} - G^a_{LL\sigma}) + G^<_{LL\sigma} \right] \tag{3}$$

where $G^{r,a,<}_{jm\sigma} = \left\langle d_{j\sigma} \mid d^+_{m\sigma} \right\rangle^{r,a<}$ denotes the retarded, advanced, and the lesser Green functions, respectively, f_α is the Fermi function, and the function Γ_α describes the coupling between the lead α and the molecule. Γ_α is proportional to the local surface density of states in the leads and the squared parameter for hopping between the molecule and leads ($v_{k\alpha}$). In what follows, Γ_α is considered to be a phenomenological constant.

Because of the presence of the Hubbard interaction in the molecular Hamiltonian H_M, it is necessary to resort to an approximative method for computing the Green functions in Eq. (3). Applying the quasiparticle approach, which is common to all first-principle calculations, we replace the molecular Hamiltonian by a single-particle form using the mean-field approximation (MFA) [26]

$$H_M \to H_M^{MFA} = \sum_{jm\sigma} t_{jm} d^+_{j\sigma} d_{m\sigma} + \sum_{j\sigma} E^{eff}_j n_{j\sigma}, \qquad E^{eff}_j = E_j + \frac{U}{2}\sum_\sigma \left\langle n_{j\sigma} \right\rangle \tag{4}$$

The non-equilibrium values of electron occupation $\left\langle n_{j\sigma} \right\rangle$ are then computed self-consistently using the lesser Green functions, $G^{r<}_{jj\sigma}$. Within the MFA, the interacting region was replaced by some effective non-interacting region with a voltage-dependent electronic structure of the Hamiltonian (4).

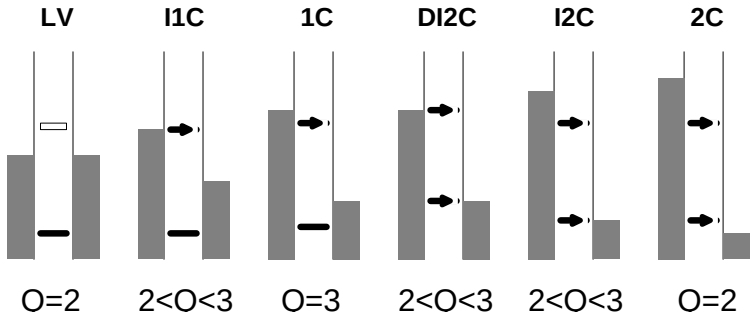

Fig. 1. Voltage ranges in the transport of a molecular junction including a 2-atom molecule. Shaded areas: occupied electron levels in the electrodes. Thick solid black lines: molecular SCE levels, fully occupied in the weak coupling limit non-contributing to the total current. Grey lines: empty and non-conducting levels in the weak coupling limit. Lines with arrows: partially occupied levels participatinge in transport. The total electron charge of the molecule in the zero coupling limit (Q) does not include an extra contribution from the voltage ramp

The main features of the voltage dependence of current in an arbitrary junction can be qualitatively understood by using a simple example of the two-atom system. The electronic structure of such a system includes just two self-consistent energy

(SCE) levels: the bonding level (E_B) and the antibonding one (E_A). In Figure 1, the subsequent voltage ranges in the transport through the 2-atom chain are indicated.

Let us discuss a typical situation for low-conducting molecular systems with weak molecule–lead coupling ($\Gamma << E_A - E_B = \Delta$) in the low temperature region ($k_BT << \Delta$). In the low-voltage (LV) range, the electrochemical potentials of the leads are usually positioned somewhere inside the HOMO-LUMO gap. In this region, and in the weak -coupling limit, the antibonding level is nearly completely empty and the bonding one is nearly completely filled and as a result the molecule is approximately neutral. The current is exponentially small in the LV region, as it requires an electron (or a hole) excitation through the gaps, $|\mu_{L,R} - E_{A,B}|$. On increasing the voltage, one of the electrochemical potentials reaches one of the SCE levels, say E_A. In the absence of electron interaction in the molecular Hamiltonian, this level would be immediately loaded by about one electron charge (in the case of symmetric coupling to both leads) and the current would exhibit a step-wise increase. The system would be in a one-channel (1C) transport range, where charge transfer between the leads does not require electron excitation.

In the presence of an electron repulsion U, the positions of the SCE levels depend on charge. When the electrochemical potential of the source lead hits the SCE antibonding level (see the second diagram in Figure 1), the process of its filling is counteracted by a corresponding rise of the level in the energy scale. In result, for finite U, the SCE antibonding level follows the position of the electrochemical potential of the source lead for some finite voltage range, and the width of this range increases with the repulsion. In this incomplete one-channel (I1C) transport range, the current grows gradually with the voltage, along with a smooth increase of the electron charge on the molecule. With a further increase in the voltage, the interacting system goes through a 1C transport range sequence and enters the I2C (incomplete 2-channel) transport range, where the electrochemical potential of the drain lead reaches the other SCE level (i.e. the bonding level in the present case). The molecule is gradually discharged and the current undergoes a second stage of rapid, but continuous increase with the voltage. This evolution ends with the 2-channel (2C) transport range, where both SCE levels are found inside the source-drain voltage window, become half -occupied (i.e. the molecule is neutral again), and the current does not increase with the voltage anymore.

The above analysis can easily be generalized to a system with an arbitrary amount of levels. The evolution of the current with changing voltage can be described as a sequence of ranges: LV...(n – 1)C–InC–nC... etc., where nC denotes the n-channel transport range. Each range with incomplete n-channel (InC) transport is characterized by a continuous increase of the current with the voltage and by an accompanying gradual charging (for odd n) or discharging (for even n) of the molecule with rising voltage. The transport ranges of fast current increase alternate with the nC ranges, where both the current and molecule charge depend on the voltage only weakly (for the weak coupling limit).

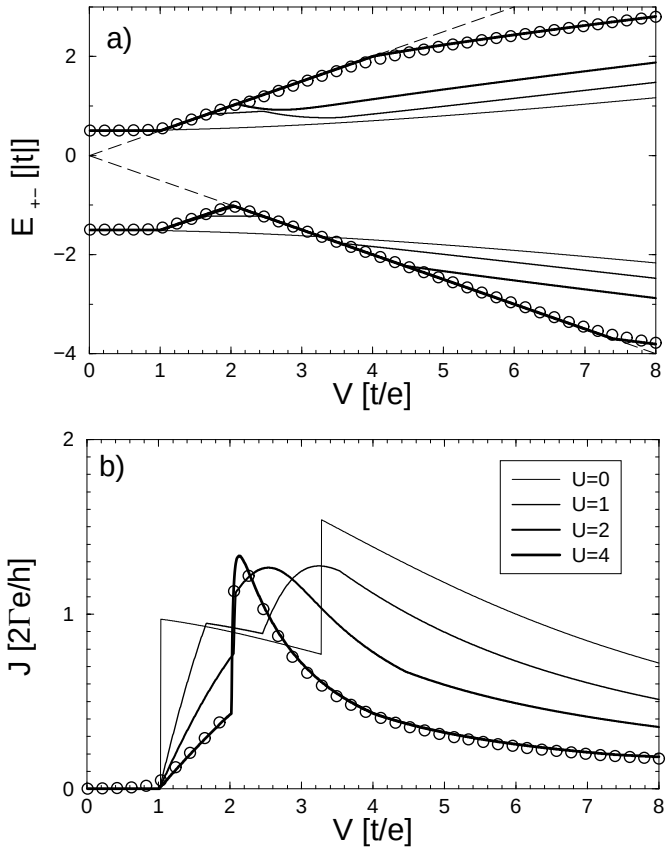

Fig. 2. Molecular junction with a 2-atom molecule: a) voltage dependence of SCE levels, as obtained from HFA for several values of Coulomb repulsion; solid lines: $\Gamma \to 0$ limit, circles: $\Gamma = 0.01$ for $U = 4.0$; all data are obtained for constant $E + U/2 = -0.5$. Broken lines denote the positions of the electrochemical potential in the leads, b) voltage dependence of the current, as obtained from HFA for several values of Coulomb repulsion; lines: $\Gamma \to 0$ limit, circles: $\Gamma = 0.01$ for $U = 4.0$; all data were obtained for constant $E + U/2 = -0.5$

In Figure 2a, we present voltage dependences of the SCE levels for the 2-atom molecule in the weak coupling limit for $E + U/2 = -0.5|t|$, whereas in Fig. 2b we show the corresponding I–V characteristics. One can see that SCE level pinning (Fig. 2a) is accompanied by a linear rise of the current (Fig. 2b) and that the slope of this rise generally decreases with increasing U for weak-to-moderate repulsion. For U strong enough ($U > 2|t|$ for $E + U/2 = -0.5|t|$), for which both SCE levels are simultaneously pinned (see the fourth diagram in Fig. 1), the current jumps rapidly and then decreases with increasing voltage; we call this range the double-incomplete 2-channel (DI2C) range. In the high voltage regime, i.e. for the 2C range, the current decreases with the voltage, which is due to the strong distortion of the SCE levels by the steep potential ramp.

3. Strongly correlated molecular junctions

The above discussion of the effects of electron interactions on transport is limited to the range of weak-to-intermediate interactions and to low temperatures. In the limit of strong on-site repulsion, the electron structure of the molecule (or a collection of coupled artificial atoms, like quantum dots) is significantly modified by such interactions [27]. In particular, the repulsion leads to an extra splitting of the one-particle peaks in the conductance spectrum, as is well known from the Coulomb blockade phenomena [22, 28].

Previous studies on transport through atomic or molecular junctions in the strongly correlated regime have usually been restricted to the weak coupling (i.e. Coulomb blockade) regime [28–30], where $\Gamma << |t|, U$. Other studies have used approximations in the sequence of the equations of motion for the Green functions, which are difficult to control [31–34]. Here, we outline a general approach that allows us to accurately reproduce the well-known limiting cases of the non-interacting model (for arbitrary values of coupling and temperature) and the strongly correlated limit of the Coulomb blockade [28, 29] (for weak coupling and not too low temperature).

We start from rewriting the molecular Hamiltonian using Hubbard operators [35]

$$H_M = \sum_{\lambda} E_{\lambda} X_{\lambda\lambda} \tag{5}$$

E_λ denotes the exact eigenvalue of the molecular Hamiltonian (in the presence of an external potential generated by the leads). The Hubbard operators are constructed using the exact eigenstates of H_M, $X_{\mu\nu} = |\mu><\nu|$. The one-particle Green functions from Eq. (3) can be written in terms of linear combinations of "mixed" Green functions, redefined in terms of Hubbard operators and single particle operators

$$G_{jm\sigma} = \sum_{\lambda\lambda'} \langle \lambda | d_{j\sigma} | \lambda' \rangle G_{\lambda\lambda',m\sigma}, \qquad G_{\lambda\lambda',m\sigma} = \left\langle X_{\lambda\lambda'} \middle| d^{+}_{m\sigma} \right\rangle \tag{6}$$

The equations of motion for the Green functions defined in Eq. (6) generate a chain of higher-order Green functions, e.g.:

$$\frac{d}{dt}\left\langle X^{F}_{\lambda\lambda'} \middle| d^{+}_{m\sigma} \right\rangle \rightarrow v_{k\alpha} \left\langle X^{B0(B2)}_{\mu\mu'} c^{(+)}_{k\alpha\sigma'} \middle| d^{+}_{m\sigma} \right\rangle \tag{7}$$

$$\frac{d}{dt}\left\langle X^{B0} c_{k\alpha\sigma'} \middle| d^{+}_{m\sigma} \right\rangle \rightarrow v_{k'\alpha'} \left\langle X^{F}_{\varsigma\varsigma'} c^{+}_{k'\alpha'\sigma''} c_{k\alpha\sigma'} \middle| d^{+}_{m\sigma} \right\rangle \tag{8}$$

where B_n indicates a boson-like Hubbard operator [36] which reduces the number of electrons in a state by n, F denotes a fermion-like Hubbard operator, which removes a single electron from a state, and $c_{k\alpha\sigma}$ is the fermion operator for the state k_σ in the lead α. In order to close the set of equations, we neglect electron correlations between the molecule and the leads and decouple the higher order Green function from Eq. (8) in the following way

$$\left\langle X^{F}_{\varsigma\varsigma'} c^{+}_{k'\alpha'\sigma''} c_{k\alpha\sigma'} \middle| d^{+}_{m\sigma} \right\rangle \rightarrow \delta_{k'\alpha'\sigma'',k\alpha\sigma'} f_{k\alpha} \left\langle X^{F}_{\varsigma\varsigma'} \middle| d^{+}_{m\sigma} \right\rangle \tag{9}$$

where $f_{k\alpha}$ is the Fermi factor. In the case of a one-atom molecule, this approximation reduces to the results of Meir et al [37] and correctly describes the limit of the Cou-

lomb blockade. In the non-interacting limit of the Hubbard model, it reproduces the exact results. For finite repulsions U, neglecting lead–molecule correlations is credible for temperatures higher than the Kondo temperature. In our numerical computation, we evaluated the poles of the Green functions in the high-temperature approximation (setting $f_{k\alpha} = 1/2$), neglecting the Kondo divergences. The residues of the Green functions can be expressed by the averages of boson-like Hubbard operators which were computed here in a self-consistent manner using appropriate lesser Green functions.

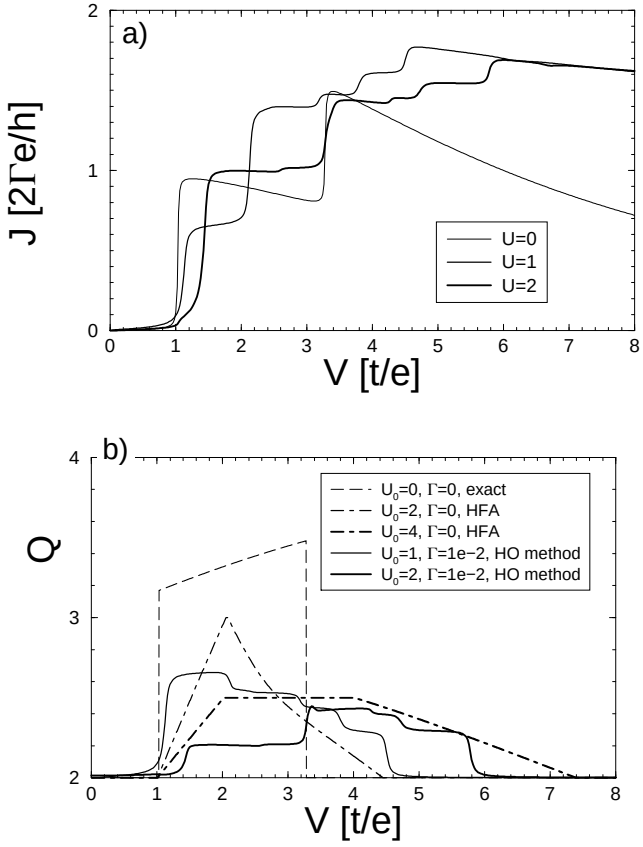

Fig. 3. Molecular junction with a 2-atom molecule: a) voltage dependence of the current, as obtained from the equation of motion method using the Hubbard operators, for several values of Coulomb repulsion for $\Gamma = 0.01$; all data were obtained for constant $E + U/2 = -0.5$; b) total electron charge as a function of the voltage, as obtained from HFA and the equation of motion method with second order decoupling

In Figure 3a, we present I–V characteristics for a junction with a 2-atom molecule, as obtained from the equation of motion approach, for several values of repulsion. One can see that the current rises in a step-wise manner with increasing voltage, unlike in the HFA computation. The electronic structure of the 2-atom molecule, with

all intramolecular electron correlations taken exactly into account, is much more complex [27] than the one obtained in the quasiparticle approach. The current steps in Fig. 3a reflect electron transitions including all excited states of the 2-atom Hubbard molecule.

In Figure 3b, we show the total electronic charge in the molecule as a function of the voltage, as obtained from both the HFA method and the equation of motion. Quantitatively, the results of both methods are similar, except for the fact that HFA tends to overestimate the value of the charge as compared to the equation of motion approach. Again, the HFA method gives a quasilinear change of the charge with voltage, which is consistent with SCE level pinning, whereas in the equation of motion method changes of the charge are step-wise.

4. Final remarks

We have analysed transport characteristics of a molecular junction including a 2-atom molecule, described by the Hubbard model. We compared the results obtained with the self-consistent quasiparticle approach (HFA) and equation of motion method, where all the intramolecular electron correlations were treated exactly and some lead–molecule correlations were neglected. While the HFA method showed SCE level pinning, accompanied by a continuous quasi-linear rise of the current for some U-dependent voltage ranges, the calculation including electron correlations does not show this effect. Concerning the charge–voltage characteristics, both methods show a suppression of the excess transferred charge Q with increasing repulsion. The observed differences are strongest for weak values of Γ, whereas for strong coupling the results of the two approaches are quantitatively and qualitatively more similar.

More theoretical work is needed to understand the role of the neglected lead –molecule correlations. One can expect that the Kondo correlations are important at least in the low temperature region and for finite charge transfer from the lead to the molecule ($Q > 2$ for $E + U/2 < 0$). Since these correlations promote the formation of resonance states at the Fermi levels of the leads, a screening of the unpaired spin of the molecule may lead to a tendency for correlated level pinning as well. In such a case, one might expect the I–V characteristics to be somewhat smoother and a region of quasi-linear increase to appear in the current–voltage dependences.

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