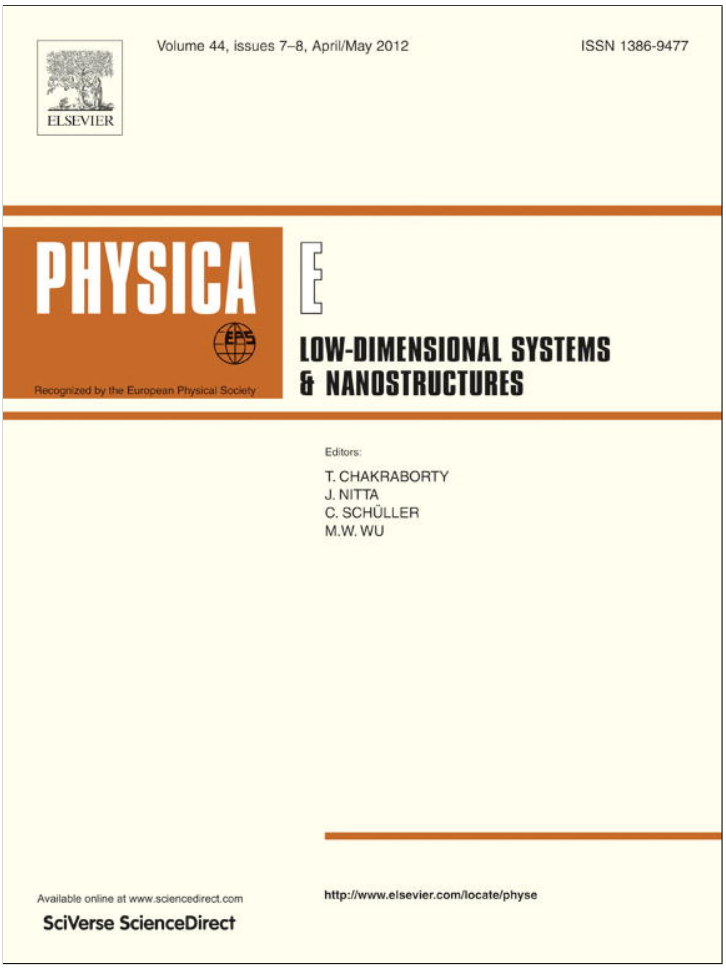

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Effect of electron–electron interaction on the transport through a nano-wire

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ABSTRACT

In this paper, a Green's function study of transport through a nano-wire in the presence of electron–electron interaction and external electric field is presented. The total Hamiltonian of the above problem is written in the tight binding approximation and Hubbard term is used to model the interaction between electrons in the central region. Our results show that in the interacting model, a conduction gap will open. Also, if the interaction between the electrons is strong enough, the negative differential resistance (NDR), which is related to the localization of charge, will not occur.

1. Introduction

Because of technological application and great underlying physics, electron transport in the molecular scale becomes an interesting topic for both experimental [1–16] and theoretical [17–27] physicist. The inclusion of different interaction into the transport problem could change conductance of nano junction. The electron–electron interaction is an interesting topic, which is still a challengeable problem for solid state physicist. Different calculations have proved that the exchange-correlation plays an important role in various properties of the solids [17,28–34]. The presence of interaction between nuclei and electrons is a complex problem in a solid. In the Born–Oppenheimer approximation the nuclear and electronic system are decoupled due to the large deference between the electron and nuclei mass. The total electronic part of Hamiltonian is written as a sum over the non-interacting part and the interaction between electrons. The existence of interaction in the Hamiltonian makes the total Hamiltonian difficult to solve. The Hubbard model is a powerful method for the investigation of electron–electron interaction in solids. It predicts metal-insulator [35–39], superfluid-insulator transitions [40–42] and superconductivity [43–46]. In the Hubbard model the presence of two electrons with different spins in the same site, increases the site potential. Due to size effect in a nano device, energy bands turn into discrete levels. The Green's function is a powerful instrument for many-body calculation in solid state physics. The non-equilibrium Green's function formalism is a well-known approach for studying quantum transport in nano devices [19,20,47–49]. The ab-initio calculations of electronic and transport properties of a nano-device are a computationally expensive, as a result parametric methods are becomes more important in the nano device calculations. In the present work, a numerical method combining the Green's function formalism and Hubbard model has been used to study the rule of electron–electron interaction in the transport properties of a typical nano-wire. The Hamiltonian of nano-wire is written in the tight-binding method and electrodes are described in the wide-band approximation. The electron–electron in the central region is explored in the mean-field Hubbard model. In the last part of article, charge distribution and current–voltage characteristic of nano-wire in the presence of an external electric field is investigated.

2. Model

Fig. 1 shows a schematic representation of a typical one-dimensional nano structure between two nonmagnetic electrodes. The total Hamiltonian of system is written as

$$H = H_w + H_L + H_R + H_T \tag{1}$$

where H_w and $H_{L/R}$ are, respectively, Hamiltonian of nano-wire and left/right electrodes. The last term in Eq. (1) describes the coupling between wire and electrodes. The Hamiltonian of nano-wire is written in the single-band tight binding model and the nearest-neighbor approximation. The electron–electron interaction in the nano-wire is studied in the Hubbard model and neglected in the both electrodes.

$$H_w = \sum_{i,\sigma} \varepsilon_i C^{\dagger}_{i,\sigma} C_{i,\sigma} + \sum_i t_i [C^{\dagger}_{i,\sigma} C_{i+1,\sigma} + C^{\dagger}_{i+1,\sigma} C_{i,\sigma}] + U \sum_i n_{i,\sigma} n_{i,-\sigma} \tag{2}$$

The two first terms in Eq. (1) show the non-interacting part of Hamiltonian, which is exactly solvable model and the third summation shows interaction between electrons. $C^{\dagger}_{i,\sigma}(C_{i,\sigma})$ is the electron creation (annihilation) operator for electron with spin σ

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Fig. 1. A schematic representation of a sandwiched nano-wire the left and right electrodes.

at site i. t_i is transfer integral between two nearest sites and ε_i is the on-site energy, which is set to zero. $n_{i,\sigma}=C^{\dagger}_{i,\sigma}C_{i,\sigma}$ is the number operator and U is the on-site coulomb interaction. We factorize the two-particle term in the Hamiltonian [50,51]. The expectation value for the number operator is calculated as [19–21]

$$\langle n_{i,\sigma}\rangle = \frac{-1}{\pi}\int_{-\infty}^{\varepsilon_f} \mathrm{Im}[G^{\sigma}_{i,i}(\varepsilon)]\ d\varepsilon \tag{3}$$

where G^{σ} the Green's function of the whole structure

$$G^{\sigma}(\varepsilon)=[(\varepsilon+i\delta^{+})I-H_w-\Sigma^{\sigma}_{L}-\Sigma^{\sigma}_{R}]^{-1} \tag{4}$$

$\Sigma^{\sigma}_{L/R}$ is the self-energy of left/right electrodes for spin σ and describes the presence of electrodes on both sides of nano-wire. Eqs. (2) and (3) are solved self-consistently and the spin density on each site is calculated. Ferretti et al., also derived a Landauer-like equation for transport in the presence of electron–electron interaction [23]. In the limit of $\Lambda=1$ current flows through nano-junction in a finite bias voltage V is calculated using the Landauer–Büttiker formula [18–20,22,23,47,48]

$$I^{\sigma}(V)=\frac{e}{h}\int T^{\sigma}(\varepsilon)[f_L(\varepsilon-\mu_L)-f_R(\varepsilon-\mu_R)]\ d\varepsilon \tag{5}$$

where $f_{L/R}$ is the Fermi function of the left/right electrode with chemical potential $\mu_{L/R}=\varepsilon_f-(eV/2)$ and Fermi energy ε_f, and T^{σ} is the transmission of electron with spin σ in the left and right electrodes

$$T^{\sigma}(\varepsilon)=Tr[\Gamma^{\sigma}_{L}(\varepsilon)G^{\sigma}(\varepsilon)\Gamma^{\sigma}_{R}(\varepsilon)G^{\sigma^{\dagger}}(\varepsilon)] \tag{6}$$

where $\Gamma^{\sigma}_{L/R}=-2\mathrm{Im}[\Sigma^{\sigma}_{L/R}]$ is the coupling matrix. For the sake of simplicity, here electrodes are described in the wide-band approximation. In this approximation, the real part of self-energy is neglected and the imaginary part is considered energy-independent. The presence of voltage difference between the left and the right electrodes produces an external electric field in the central region. In this situation, the total Hamiltonian of nano-wire becomes $H_w \rightarrow H_w+H_E$. The Hamiltonian of the electric field, which is assumed uniform along the molecule, is written as

$$H_E(V)=\sum_{i,\sigma}\left(\frac{V}{L}\right)\left[\frac{L}{2}-X(i)\right]C^{\dagger}_{i,\sigma}C_{i,\sigma} \tag{7}$$

where L is the wire length and $X(i)$ is the position of i-th atom. The presence electric field changes the electronic structure and charge distribution of nano-wire. In this situation, the total Hamiltonian and transmission become voltage dependent.

3. Results

In this section we focus on the transmission and current–voltage curves of a typical nano-wire. Throughout this article, we shall describe all the essential features of transport in the non-interacting, week interaction and strong interaction regime. We consider a nano-wire with 7 atoms and set $t=3$ eV, $U=0$, t, $2t$ and $\Gamma^{\sigma}_{L/R}=0.5$ eV. Fig. 2 shows the transmission and current–voltage characteristics of a nano-wire in the non-interacting and Hubbard model. Because of the nano scale dimensional of wire, transmission curve finds peaks in the energy eign-value of single wire. By increasing the applied voltage, new states enter to the energy window and current increases. As a result, the current–voltage characteristic of the nano-wire finds a step-like shape, which is observed in previous experimental works [1–6]. The shape of current steps depends on the height and distance between resonant levels in the transmission curve and reflects the electronic structure of nano-wire. The coupling strength between molecule and electrodes is an important factor, which changes the

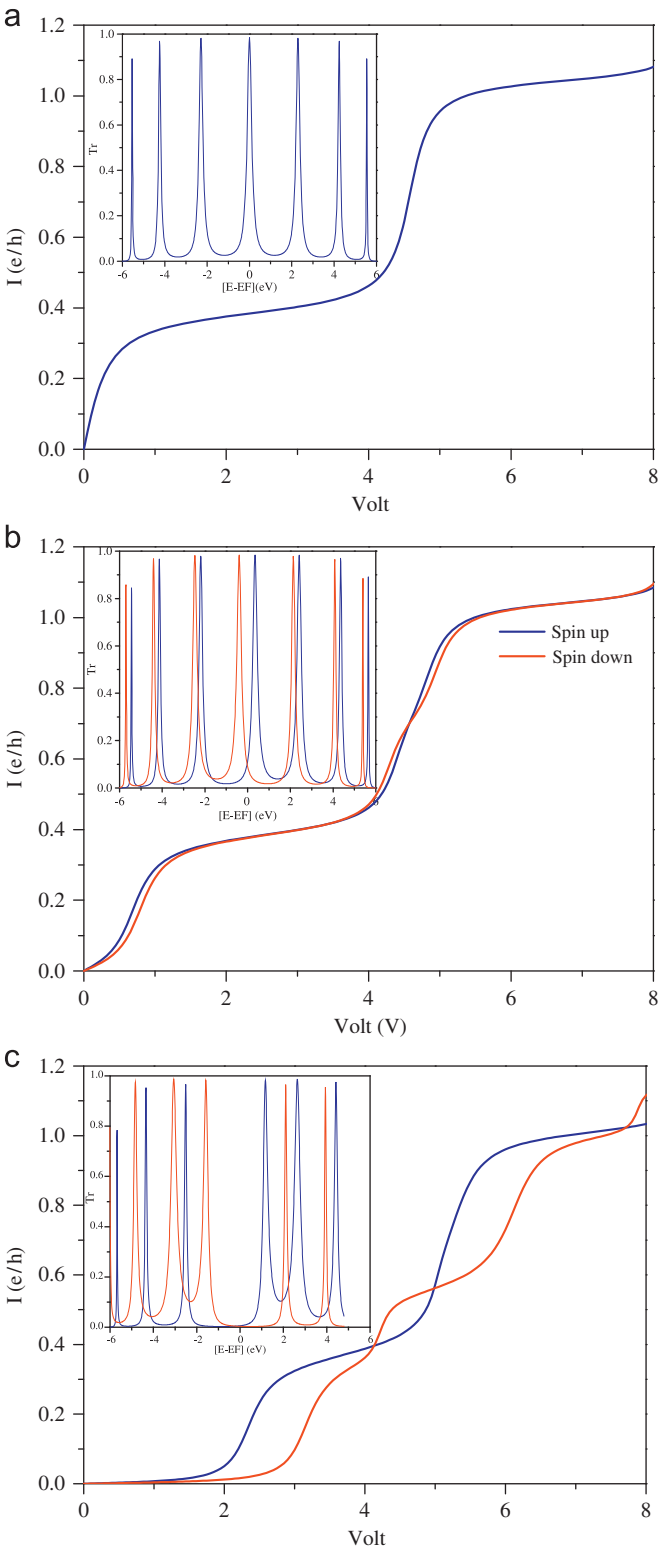

Fig. 2. Transmission and the current–voltage curves for spin-up and down in the (a) non-interacting ($U=0$) and Hubbard model with (b) $U=t$, (c) $U=2t$.

transmission and current voltage characteristic considerably [24–27]. In the case of non-interacting model ($U=0$) transmission for spin-up and spin-down are identical. Due to the electron–electron interaction in the central region, there is an energy gap between highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of spin-up and down. In the interacting model one can find the transmission for spin-up and down is not degenerate. By increasing the interaction strength, the transmission curve for different spins splits and conductance gap appears at the Fermi level, which shows the metal-insulator transition caused by the Hubbard interaction. The presence of the transmission gap in the interacting model leads to a threshold voltage in the current curve. In the Hubbard model, the transmission peaks near to the Fermi level are related to the spin-up LUMO and spin-down HOMO states. the transmission peak corresponding to spin-up LUMO will first enter into the energy window, which means that in lower voltage region total current is dominated by spin-up electrons. So the interaction strength significantly changes the electron transport through a typical nano-junction. By considering the presence of external electric field in the non-interacting model, electrons accumulate in one side of the nano structure [18,22]. However, in the Hubbard model, the presence of the electric field accompanied with the Hubbard interaction leads to a complex spin distribution in the nano structure, which is shown in Fig. 3. In the nano-wire, each site collects different spin and spin population is reversed in higher voltage. Sum over the spins density shows the charge distribution of each site. The deference between the spin-up and down on each site is related to the magnetic moment of site in the presence of external electric field in an interacting nano-device. The complex behavior of spin density along the nano-wire produces an effective internal potential. Fig. 4 shows the total current–voltage curve in presence of external electric field in the non-interacting and Hubbard model. By increasing the strength of interaction, the current decreases and at higher strength shows semi-Ohmic behavior in higher voltages. Although increasing the applied voltage opens the energy window, charge localization, caused by the external electric field, decreases current through the nano structure. As a result, in the non-interacting model, a competition between these phenomena produces a negative slope in the current–voltage curve called negative differential resistance (NDR). By adding the Hubbard term to the total Hamiltonian in the presence of electric field, the repulsion between electrons changes the result of the above competition. If the interaction between electrons is strong enough, the electric field is screened and NDR does not occur in the interacting model. Thus, the electron–electron interaction produces an effective

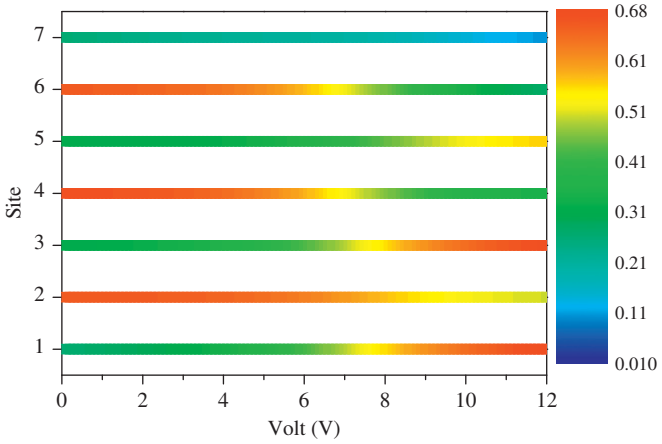

Fig. 3. Spin-up distribution in the interacting model with $U=2t$.

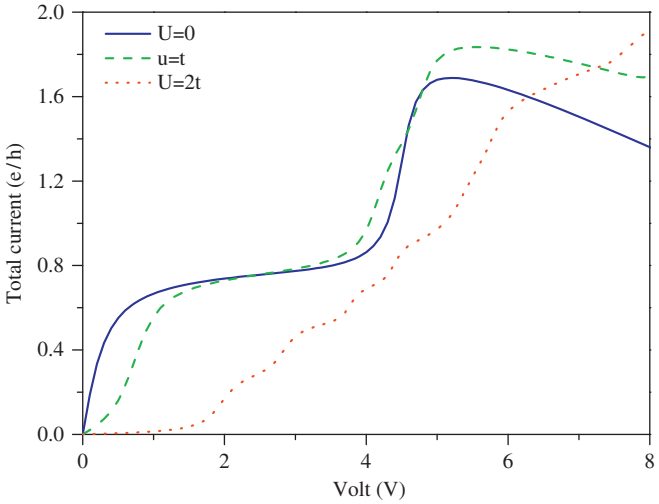

Fig. 4. Total current in the presence of an external electric field.

internal potential, which could counteract the effects of an external electric field. The results show the origin of NDR, which was observed in previous experimental works [2,5–10]. Also, the inclusion of interaction between electrons explains the non-presence of NDR in all nano-devices [1,11–16].

4. Conclusion

In summary, we studied the transport through a typical one-dimensional nano device in the presence of the electron–electron interaction and the external electric field using tight binding method. The interaction between electrons is studied in the mean-field Hubbard model. The presence of interaction induces splitting between transmission curves for electrons with spin-up and down. Also, the existence of an external electric field in the central region is investigated. Our results demonstrate the NDR as a consequence of voltage damping in the central region. According to the results, if the electron–electron interaction is strong enough, it will produce an internal field, which screen the external electric field and cancel NDR. Our results confirm the importance of many-body interactions in the transport properties of a typical nano-device.

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