MANY BODY EFFECTS ON THE TRANSPORT PROPERTIES OF A DOPED NANO DEVICE

M. Modarresi[1*], M. R. Roknabadi[1], N. Shahtahmasbi[1], M. Mirhabibi[2]

1 Department of Physics, FerdowsiUniversityof Mashhad, Mashhad Iran.
2 Payame Noor University ofKerman

ABSTRACT

In this article, we study the effect of electron-electron interaction in a doped nano cluster sandwich between two electrodes. The Hamiltonian of the cluster is written in the tight-binding model and electrodes are described in the wide-band approximation. The GW approximation has been used for the calculation of the exchange-correlation term in the cluster region. Our results showed that in the presence of the electron-electron interaction the transmittance gap increases and current decreases. Also, in a doped nano structure the transmission decreases and many body effect becomes more important. By considering the exchange-correlation in a doped nano cluster in the GW approximation the transmission and current decrease drastically.

Keywords: nanocluster; doping; many body theory; transport properties.

INTRODUCTION

Transportation through a nano device is an interesting topic for theoretical and experimental physicist [1-4]. In realistic systems the impurity effects are Inevitable. The presence of an impurity in a nano system changes the electronic and transport properties of the device. In the one particle approach and in a tight binding approximation the Hamiltonian of cluster is written according to the on-site and hopping term between nearest neighbors in the cluster. In this approach the the impurity effects are limited in the change of tight binding parameters. But due to the electron-electron and electron-phonon interactions in the nano device, we face a complex many-body problem. The effect of electron-phonon interaction has been studied in previous works[5-8]; in this article, the effect of electron-electron interaction in a doped nano device is studied. The electron-electron interaction plays an important role in solids and responsible for the coulomb blockade and the Kondo effects [9]. Based on the Born-Openheimer approximation, the electronic and the ionic degrees of freedom are decoupled. The Hartree and Hartree-Fock (HF) methods try to deals the electron-electron interactions as a one-particle term in the total Hamiltonian. The Hartree method simply adds the classical repulsion to the one particle Hamiltonian. In the GW approximation the self-energy is approximated with the first

* e-mail: mo_mo226@stu-mail.um.ac.ir tel: +98-9133452131

term in the expansion. Many body effects beyond the GW approximation could be important in the calculation of different properties of solids [10-12] but the GW approximation is reliable in different calculations [1, 3, 13-15]. The HF approximation contains the classical electrostatic and exchange potentials but the GW approximation includes the correlation between electrons in solids [16]. In this work we investigate the many body effect in a doped nano cluster.

MODEL AND RESULTS

We consider a typical nano cluster with 6 atoms and attach the left and right electrodes to the cluster, as shown in *Figure 1*. At first the transport in a pure and doped cluster in a one-particle approach has been investigated. The total Hamiltonian of the above system contains the Hamiltonian of isolated cluster, electrodes and the interaction between them.

Fig. 1– A pure and doped nano cluster with 6 point between two electrodes

The non-interacting part of the Hamiltonian is written in the nearest neighbor tight-binding approximation as follows,

$$H_{0C} = \sum_{i,\sigma} \varepsilon_i C^{+}_{i,\sigma} C_{i,\sigma} - t_i (C^{+}_{i+1,\sigma} C_{i,\sigma} + C^{+}_{i,\sigma} C_{i+1,\sigma}) \qquad (1)$$

The index i runs over the cluster sites. The operator$C_{i,\sigma}^{+}(C_{i,\sigma})$ creates/annihilates a π electron with spin σ at the i-th site of cluster. εi is the onsite energy of the i-th sites and ti denotes the hopping integral between two neighboring sites. The effect of electrodes on the Hamiltonian is fully described by specifying the self-energy of the left and right electrodes. By using the Keldysh Green's function technique, the current running between two electrodes, through the cluster, is calculated by Meir-Wingreen relation [2, 17]. Neglecting the interaction in the central region, the Mier-Wingreen relation is simplified to the well-known Landauer-Büttiker formula [18, 19],

$$I(\mathrm{V_B}) = \frac{e}{h} \int_{-\infty}^{+\infty} d\omega \, T(\omega) [f_L(\omega) - f_R(\omega)] \qquad (2)$$

Where $f_{L/R} = [\exp[\beta(\omega - \mu_{L/R})] + 1]^{-1}$ is the Fermi distribution function in the left/right electrode with chemical potential $\mu_{L/R} = \varepsilon_f \pm (eV_b/2)$ and Fermi energy ε_f. $T(\omega)$ is the transmission coefficient as a function of energy for electrons and can be written as follows,

$$T(\omega) = Tr[\Gamma_L G_0^r(\omega)\Gamma_R G_0^a(\omega)], \quad (3)$$

where $G_0^r(\omega)$ is the retarded Green's function of the non-interacting system and is defined as,

$$G_0^r(\omega) = [\omega \mathrm{I} - H_{0C} - \Sigma_L - \Sigma_R]^{-1} \quad (4)$$

$\Gamma_{L/R}$represents the coupling between the cluster and left/right electrode. In this article, the spin-flip process has been neglected and the self-energy of electrodes has been simply described within the wide-band approximation. In this approximation, the real part of self-energy is neglected and the imaginary part of the self-energy operator is written in an energy-independent form as [5, 20], $\sum_{L/R}=(-i/2)\Gamma_{L/R}$. In the pure cluster we set $\varepsilon_i=0$, $t_i=3.0$ev,and in the doped cluster for the dopant site we use $\varepsilon_d = -1$, $t_d = 2$ev, and electrodes described with the following parameters, $\Gamma_L = \Gamma_R = 0.066$ t0. *Figure 2* shows the current voltage characteristic and transmission as functions of energy for the above clusters. In both cases the transmission peaks are correspondent to the eigenvalue of the non-interacting system.

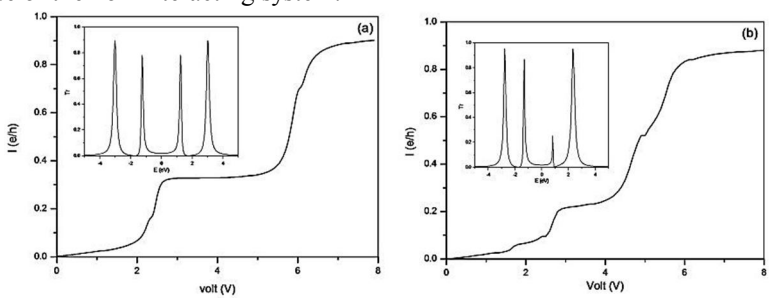

Fig. 2– Current volt-voltage characteristic and transmission as a function of energy for the case of (a) pure and (b) doped nano cluster

The symmetry around the Fermi energy in the pure cluster is due to the symmetry of the Hamiltonian in the pure cluster. In the doped structure the symmetry around the Fermi energy vanishes. By increasing the applied voltage the energy window opens and the current increases. When a transmission peak enters in the energy window, current increases more rapidly which leads to a step-like form in the current-voltage curve. In the next step, we consider the interacting cluster and study the effect of electron-electron interaction on the

transport properties of a pure and doped 2D cluster in the Hartree and G_0W_0. The quasi-particle equation for interacting electrons can be written as [21, 22],

$$[H_{0C} + V_H]\Psi_i(r) + \int \Sigma(r, r', \varepsilon_i)\Psi_i(r')\, dr' = \varepsilon_i \Psi_i(r) \tag{5}$$

Where V_H is the electrostatic or Hartree potential of the electronic system and Σ is the self-energy which is a non-local, energy-dependent and non-hermitian operator containing all exchange and correlation effects beyond the Hartree approximation. In the GW method, the time-ordered self-energy operator is approximated as [1, 23, 24],

$$\Sigma_{GW}(r, r', \omega) \simeq \frac{i}{2\pi} \int_{+\infty}^{-\infty} d\omega'\, W(r, r', \omega')\, G(r, r', \omega - \omega')\, e^{-i\omega'\delta} \tag{6}$$

Where G is the one-particle Green's function, W is the dynamically screened coulomb interaction and δ is a positive infinitesimal. The GW method can be considered as a generalization of the HF approximation, in which the bare coulomb interaction $\upsilon(r, r') = 1/|r - r'|$ is replaced with the dynamically screened interaction W. In this article, the Green's function is approximated with the non-interacting Green's function [16, 22, 25]. The screened interaction can be calculated in terms of the inverse dielectric function ε^{-1} by means of,

$$W(r, r', \omega) = \int dr'\, \varepsilon^{-1}(r, r'', \omega)\, \upsilon(r, r'') \tag{7}$$

In the direct space, the dielectric function can be written as $\varepsilon = 1 - \upsilon P$. In its simplest form, the polarization operator P can be written in the independent particle approximation as [25],

$$P(r, r', \omega) = \sum_{i,j} (f_i - f_j) \frac{\Psi_i(r)\, \Psi_j^*(r)\, \Psi_j(r')\, \Psi_i(r')}{\omega - (\varepsilon_j - \varepsilon_i) + i\eta} \tag{8}$$

Where; f_i is the occupation of the i-th state and iη is a small imaginary part which leads to an imaginary part of P. The above equation for polarization is the form of the random-phase approximation (RPA) first used by Lindhard for the homogeneous electron gas [26, 27]. The imaginary part has peaks in $\delta(\varepsilon_j - \varepsilon_I - E)$ which shows the conservation of energy in case of excitation of an electron from state i to state j. The retarded Green's function can be written as,

$$G_C^r(\omega) = [\omega I - (H_{0C} + V_H - \Sigma_L^r - \Sigma_R^r - \Sigma_{GW}^r(\omega)]^{-1} \tag{9}$$

Where Σ_{GW}^r is the retarded self-energy operator due to the electron-electron interaction. A. Ferretti and et al. proposed a Landauer-like expression for current in the presence of many-body interactions as follows[2],

$$I^{\sigma,\sigma'}(\mathrm{V_B}) = \frac{e}{h}\int_{-\infty}^{+\infty} d\omega\, Tr\,[\Gamma_L^r G_C^r(\omega)\Gamma_R^r \Lambda G_C^a(\omega)][f_L(\omega) - f_R(\omega)] \qquad (10)$$

We set $\Lambda = 1$ and restrict the changes in the definition of the retarded Green's function which is correspondent to the strong coupling with electrodes. *Figure 3* shows the transmission as a function of energy in the Hartree and GW approximations.

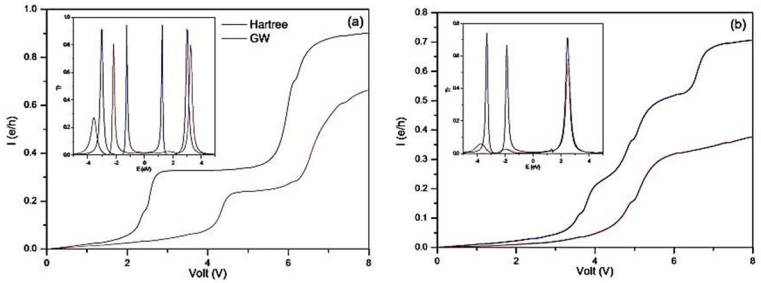

Fig. 3– Current volt-voltage characteristic and transmission as a function of energy in the Hartree and GW approximation for the case of (a) pure and (b) doped nano cluster

In the Hartree approximation, the H_0 in the equation 4 is replaced with $H_0 \to H_0 + V_H$. In the Hartree model the transmission spectrum in the pure cluster does not change. But the transmission for the doped cluster decreases and transmission gap increases with respect to the non-interacting case. A comparison between the Hartree and GW appears the many body effects in the cluster region. In the GW approximation the real part of self-energy shifts the transmission peaks and increases the conductance gap. The imaginary part of self-energy leads to decreasing transmission and broadening in the transmission peaks. Figure 3 shows the current-voltage characteristic of the cluster in Hartree and GW approximation. The exchange-correlation term described in the GW approximation decreases the transmission and current which is correspond with an additional resistance in the cluster. In the doped nano cluster the electrons are accumulate in the dopant site. As a result the many body effect becomes more important in a doped cluster, thus the transmission reduces drastically in the GW approximation.

CONCLUSIONS

Briefly speaking, we have considered a typical nano structure and have studied the effect of electron-electron interaction on the transport properties in Hartree and GW approximations. Our results showed that in the presence of e-e interaction, conductance gap increases and current decreases. The reduction of transmission and current is increases in a doped cluster.

Acknowledgements

We would like to express our gratitude to Dr. Andrea Ferretti, Dr. KristianSommerThygesen, and Dr. Mikkel Strange for their useful consultations.

REFERENCES

[1] P. Darancet, A. Ferretti, D. Mayou, and V. Olevano, Phys. Rev., B 75 (2007) 075102.
[2] Ferretti, A. Calzolari, R. Di Felice, and F. Manghi, Phys. Rev., B 72 (2005) 125114.
[3] K. S. Thygesen, Phys. Rev. lett.,100 (2008) 166804.
[4] Q. Yu, L. A. Jauregui, W. Wu, R. Colby, J. Tian, Z. Su, H. Cao, Z. Liu, D. Pandey, D. Wei, T. F. Chung, P. Peng, N. P. Guisinger, E. A. Stach, J. Bao, S.-S. Pei, and Y. P. Chen, Nat. Mater.Advan.online public.,2011.
[5] M. Modarresi, M. R. Roknabadi, N. Shahtahmasbi, D. VahediFakhrabad, and H. Arabshahi, Phys. B,Conden. Matt., 406 (2011) 478.
[6] M. Pourfath and et al., J. of Phys., Conference Series, 109 (2008) 012029.
[7] K. Walczak, Chem. Phys., 333 (2007) 63.
[8] Z.-Z. Chen, Rong, and B.-f. Zhu, Phys. Rev., B 71, (2005) 165324.
[9] J. Park, A. N. Pasupathy, J. I. Goldsmith, C. Chang, Y. Yaish, J. R. Petta, M. Rinkoski, J. P. Sethna, H. D. Abruna, P. L. McEuen, and D. C. Ralph, Nature, 417 (2002) 722.
[10] P. Sun and G. Kotliar, Phys.Rev.Lett., 92 (2004) 196402.
[11] M. G. Vergniory, J. M. Pitarke, and P. M. Echenique, Phys. Rev., B 76 (2007) 245416.
[12] P. Romaniello, S. Guyot, and L. Reining, J. of Chem.Phys., 131 (2009) 154111.
[13] G. Pal, Y. Pavlyukh, H. C. Schneider, and W. Huebner, European Phys.J. B-Condensed Matter and Complex Systems, 70 (2009) 483.
[14] X. Wang, C. D. Spataru, M. S. Hybertsen, and A. J. Millis, Phys. Rev. B, 77 (2008) 045119.
[15] K. S. Thygesen and A. Rubio, Phys. Rev., B 77 (2008) 115333.
[16] J. C. Inkson, Cavendish Lab., Univ. of Cambridge, Cambridge, 1984.
[17] Z. Z. Chen, R. Lü, and B. Zhu, Phys.Revi., B 71 (2005) 165324.
[18] H. D. Cornean, A. Jensen, and V. Moldoveanu, J. of Math.Phys., 46 (2005) 042106.
[19] D. S. Fisher and P. A. Lee, Phys. Rev., B 23 (1981) 6851.
[20] P. Cui, X.-Q. Li, J. Shao, and Y. Yan, Phys.Lett., A 357 (2006) 449.
[21] V. I. Anisimov, F. Aryasetiawan, and A. Lichtenstein, J. of Phys, Condensed Matter, 9 (1997) 767.
[22] P. Garcia-Gonzalez and R. Godby, Comp.Phys. Commun., 137 (2001) 108.
[23] N. Hamada, M. Hwang, and A. Freeman, Phys. Rev., B 41 (1990) 3620.
[24] T. A. Niehaus, M. Rohlfing, F. Della Sala, A. Di Carlo, and T. Frauenheim, Phys. Rev., A 71 (2005) 022508.
[25] G. Onida, L. Reining, and A. Rubio, Rev. of Mod. Phys., 74 (2002) 601.
[26] K. D. V. S. M. F. M. J. Lindhard, 8 (1954),
[27] N. D. Mermin, Phys. Rev., B 1 (1970) 2362.