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The effect of electrical impurity on quantum conductance in a simple cubic nano-wire

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Abstract

In the present work, the effect of a central electrical impurity (dipole) on quantum conductance in simple cubic nano-wires (SCNW) has been investigated in the tight-binding (TB) approach and assuming nearest-neighbor interaction by Green's function (GF) method. We illustrate that in the presence of electrical impurity (external potential), the number of channels and energy band of nano-wire decrease. The variation of the energy band and the number of channels depend on the position and amount of the electrical charge (dipole moment) in the SCNW.

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1. Introduction

The study of electrical conductance in mesoscopic systems is one of the most fundamental problems in nanostructure physics. In recent years, there has been a growing interest in electrical transport in quantum dots (QDs), quantum wires, and molecular wires [1–5]. Several different methods have been developed for the study of electron-impurity potential scattering that have a common basis in the Landauer [6–9] approach. In this approach, in the linear response regime, the conductance is obtained as a quantum mechanical problem and can be related to the total transmission at the Fermi energy, on the other hand, $G = (2e^2/h)T(\varepsilon_F)$. We rely on this theory as the basis for studying the conductance properties of nano-wire systems in the presence of an electrical impurity.

In our previous works, we have calculated theoretically the coherent conductance, resonant and bound state energies in the TB approach and assuming nearest-neighbor interaction for uniform nano-crystal [10], periodic QD [11], molecular wire [12], and general periodic nanostructure [12] systems by Green's function (GF) and transfer matrix methods.

In the present paper, we study the quantum transport in a simple cubic QD (SCQD) attached to the metallic nano leads in the ballistic regime. In Section 2, we investigate the relation between GF and the electrical conductance for a general nanostructure system. In Section 3, we study the effect of a central electrical impurity and an electrical dipole on coherent conductance. Finally, the paper is ended with a conclusion.

2. Theoretical model

We assume the isolated system A has been introduced with H_A Hamiltonian in tight-binding (TB) approach. For this system the GF is defined as follows:

$$(\varepsilon I - H_A)G_A = I, \tag{1}$$

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where ε, I and, G stand for energy, unit operator and the GF operator for isolated system A, respectively. Now, we assume a system divided into two subsystems A and B, the Hamiltonian for the whole system is considered as follows:

$$H = H_{\mathrm{A}} + H_{\mathrm{B}} + H_{\mathrm{int}}, \tag{2}$$

in which H_{int} refers to the Hamiltonian of the interaction between two subsystems A (such as QD) and B (such as left or right lead), with regard to GF definition, the GF inverse of system A in the presence of system B and vice versa are as [3,10]

$$\begin{aligned} G_{\mathrm{A}}^{-1}(\varepsilon) &= G_{\mathrm{A},0}^{-1}(\varepsilon) - H_{\mathrm{int}} G_{\mathrm{B}}(\varepsilon) H_{\mathrm{int}}, \\ G_{\mathrm{B}}^{-1}(\varepsilon) &= G_{\mathrm{B},0}^{-1}(\varepsilon) - H_{\mathrm{int}} G_{\mathrm{A}}(\varepsilon) H_{\mathrm{int}}, \end{aligned} \tag{3}$$

where $G_{\mathrm{A(B)}}^{-1}(\varepsilon)$ and $G_{A(B),0}^{-1}(\varepsilon)$ are the GF inverse of subsystem A (B) in the presence of subsystem B (A), the GF of isolated system A (B) and interaction Hamiltonian between two systems A and B, respectively. It can be seen from Eq. (3), the two mentioned GFs are related to each other. Thus, for calculating GF of system A, we need to calculate the GF of system B and vice versa. Now, we assume that the comprising cells/particles of system B are much more numerous than system A, in this case, subsystem A, will not cause a considerable change in the energy band of system B, but, the energy spectrum of subsystem A changes in the presence of system B, which this changes are depended on H_{int} term. Therefore, with respect to the above reasoning the GF of subsystem B is independent of presence or absence of subsystem A, then, the GF of system A in the presence of system B becomes

$$G_{\mathrm{A}}^{-1}(\varepsilon) = G_{\mathrm{A},0}^{-1}(\varepsilon) - H_{\mathrm{int}} G_{\mathrm{B},0}(\varepsilon) H_{\mathrm{int}}, \tag{4}$$

in which the second term in Eq. (4) is called the system A self-energy in the presence of subsystem B. On the other hand, in general form, the self-energy operator is introduced as follows:

$$\Sigma_{\mathrm{A}}(\varepsilon) = H_{\mathrm{int}} G_{\mathrm{B},0}(\varepsilon) H_{\mathrm{int}}. \tag{5}$$

In the meanwhile, the system A could physically be an atom, molecule, polymer, atomic cluster or even a superlattice with nanometer dimensions, and in the case of system B it can be a nano-electrode, nano-tube or sort of a long length carbon chain (molecule wire).

3. Conductance of a simple cubic nano-wire: GF approach

Now, we consider a nano-wire composed of a SCQD attached to two uniform simple cubic nano-leads. For simplicity, two metallic leads are assumed ideal.

Also we calculate the electrical conductance in the coherent mechanism. It means that the dot length is smaller than the phase coherence length. The whole system Hamiltonian including the QD, contacts and leads Hamiltonians are introduced as

$$H = H_{\mathrm{L}} + H_{\mathrm{DL}} + H_{\mathrm{D}} + H_{\mathrm{DR}} + H_{\mathrm{R}}, \tag{6}$$

where $H_{\mathrm{L,D,R}}$ describes the Hamiltonian of the left-lead, the dot, and the right-lead, and also, $H_{\mathrm{DL(R)}}$ refers to the interaction Hamiltonian between the QD and the left (right) lead. In the other words, the terms H_{D}, $H_{\mathrm{L(R)}}$ and $H_{\mathrm{DL(R)}}$ in Eq. (6) are replaced with H_{A}, H_{B} and H_{int}, respectively, in Eq. (2).

Here for simplicity, we assume that the geometry of the quasi-one-dimensional system is simple cubic, assuming a simple cubic QD with $N_x \times N_y \times N_Z$ atoms which is coupled to the simple cubic nano-wire with $N_x \times N_y$ atoms in cross-section, also, both the dot and leads are assumed to have the same geometry. Fig. 1 shows a schematic of typical simple cubic dot (SC-DOT) where is attached to the simple cubic leads.

We further assume that all the hopping integrals, from one unit cell to the next, are the same regardless of atom positions within the unit cell, but the onsite energies need not to be the same within a cell, or from one unit cell to the next in the dot region.

We have obtained a unitary transformation which separates different modes of this system in Ref. [10]. In this reference we have showed the quasi-one-dimensional (simple cubic nano-wire (SCNW)) problem with $N_x \times N_y$ atoms in xy arrangement (cross-section of the SCNW), converts to the $N_x \times N_y$ number of one-dimensional chains problem without interaction, but, with different on-site energies depended on mode numbers. Following the mentioned unitary transformation, the SCNW Hamiltonian can be written as

$$H_{\alpha} = \sum_{m,n,j} \varepsilon_{\alpha,mn} c_{mn,j}^{+} + \sum_{mn,j} t_{\mathrm{D(R)}} \left(c_{mn,j}^{+} c_{mn,j+1} + \mathrm{h.c.} \right), \tag{7}$$

where α refers to the L (left-lead) or R (right-lead) or D (dot), j refers to the site index (cell number) in the z-axis direction. Also the mode number m (n) refers to quantum number in xy cross-section after diagonalization, and $t_{\mathrm{D(R)}}$ refers to the hopping term in z-axis direction. In Eq. (7) the on-site energies for the left and right leads are derived as

$$\varepsilon_{\mathrm{L(R)},mn} = 2t_{\mathrm{L(R)}x} \cos\left(\frac{m\pi}{N_x + 1}\right) + 2t_{\mathrm{L(R)}y} \cos\left(\frac{n\pi}{N_y + 1}\right), \tag{8}$$

where $t_{\mathrm{L(R)}x}$ and $t_{\mathrm{L(R)}y}$ refer to the hopping term in the cross-section of the leads in the x and y direction, respectively.

The interaction Hamiltonian between the QD and the left and right leads in the TB approach and nearest-neighbor

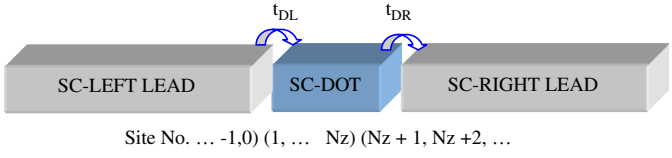

Fig. 1. Schematic of a typical SCNW (simple cubic dot attached to the simple cubic leads).