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Analytical results on coherent conductance in a general periodic quantum dot: Transfer matrix method

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Abstract

In this work, we study the conductance of a general periodic quantum dot (QD) attached to ideal semi-infinite uniform metallic leads (nanocrystals), fully analytically. We propose a new general formula which relates conductance to transfer matrix (TM) for an isolated cell in the periodic dot. The equation describes exactly the dependence of the transmission coefficient (TC) on Fermi energy, dot-size, dot–lead coupling, and gate voltage for an arbitrary periodic dot. Then, we derive a nonlinear equation which gives the resonance, bound, and surface state energies. Finally, the TC has been calculated for gapless, single, and double gap models exactly. Moreover, we have also calculated the effects of the cross-section of the leads, which were separated by a polymer chain on the conductance. Our calculations can be generalized to any type of QD and quantum wire (QW) within the one-electron approximation, and, can be applied to, e.g., molecular, polymer, and nanocrystal junctions, where these results may be useful in designing future molecular electronic devices.

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1. Introduction

In the past few years, the study of electronic transport through quantum dots (QDs), quantum wires (QWs), and molecular wires have been major areas of research in mesoscopic physics [1–3]. The size and shape of QDs and QWs can be precisely controlled with today's technology [1,2,4]. QDs can be connected to electrodes and are, therefore, excellent tools to study atomic-like properties. The transport properties of a QD can be measured by coupling it to leads and passing current through the dot. In fact, there is a vast and recent literature on this subject [1–3]. Here, at low temperatures, we ignore the inelastic scattering process, thus, conductance through a QD is characterized by quantum coherence. We rely on the Landauer's approach [5] for studying the coherent transport properties in QD and QW systems. The Landauer's approach states that electronic conductance is proportional to transmission coefficient (TC). Different methods based on this approach have been developed for the study of transport phenomena. One class of methods is based on the transfer matrix (TM), e.g. [1,3,6–12], and the others make use of Green's function (GF) formalism, e.g. [3,13–20].

In our previous works [20], we have calculated the coherent conductance for uniform and alternating dot fully analytically by GF method. In the present paper, we use an analytical method based on the tight binding (TB) model and transfer matrix method to derive dependence of conductance on Fermi energy, dot-size, and gate voltage, for a general periodic dot connected to two uniform ideal leads at $T = 0\,\mathrm{K}$.

The organization of this paper is as follows. In Section 2, the TB one-electron Hamiltonian for a general QD is described. Here, a detailed description of the TM approach in the TB model, assuming nearest-neighbor interaction, is given. In this section, for a general dot, the TC, which depends on the Fermi energy, QD size, dot–leads coupling, and gate voltage was derived analytically. The TC calculations in the periodic dot case are explained in much detail in Section 3. Also, in this section we obtain a nonlinear equation which gives the resonant and bound states energies and surface state energies if they exit. In Section 4, we calculate the TC for gapless, single gap, and double gap dots in more details. The paper ends with the conclusion in Section 5.

2. Description of transfer matrix method

We consider a chain composed of a general QD attached to two uniform semi-infinite leads. For simplicity, the two metallic leads are assumed to be ideal. Also, the elements of TM for the general QD are calculated by coherent mechanism. It means that the dot length is smaller than the phase coherence length [3]. The generalized Hamiltonian which describes the system is given by

$$H = H_{\mathrm{L}} + H_{\mathrm{DL}} + H_{\mathrm{D}} + H_{\mathrm{DR}} + H_{\mathrm{R}}, \tag{1}$$

where $H_{\mathrm{L,D,R}}$ describes the Hamiltonian for the left lead, dot and the right lead, and also, $H_{\mathrm{DL(R)}}$ refers to the Hamiltonian for the coupling between the general QD and the left (right) lead. The Hamiltonian of left (right) lead is defined as

$$H_{\mathrm{L(R)}} = t_{\mathrm{L(R)}} \sum_i (c_i^{\dagger} c_{i+1} + \mathrm{h.c.}), \tag{2}$$

where $t_{\mathrm{L(R)}}$ refers to the hopping integral between s atomic orbitals (assumed to be orthogonal), for the left and right lead, i varies between $(-\infty, 0]$ and $[N+1, +\infty)$, respectively, and N refers to the number of total atoms in the dot. The QD is coupled to the leads via the contact Hamiltonian, $H_{\mathrm{DL(R)}}$ as follows:

$$H_{\mathrm{DL(R)}} = t_{\mathrm{DL(R)}} (c_{0(N)}^{\dagger} c_{1(N+1)} + \mathrm{h.c.}), \tag{3}$$