Coherent transport in linear arrays of quantum dots: the effects of period doubling and of quasi-periodicity

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Abstract

We evaluate the phase-coherent transport of electrons along linear structures of varying length, which are made from two types of potential wells set in either a periodic or a Fibonacci quasi-periodic sequence. The array is described by a tight-binding Hamiltonian and is reduced to an effective dimer by means of a decimation-renormalization method, extended to allow for connection to external metallic leads, and the transmission coefficient is evaluated in a $T$-matrix scattering approach. Parallel behaviors are found for the energy dependence of the density of electron states and of the transmittivity of the array. In particular, we explicitly show that on increasing its length the periodic array undergoes a metal-insulator transition near single occupancy per dot, whereas prominent pseudo-gaps emerge away from the band center in the Fibonacci-ordered array.

Key words: Coherent one-dimensional transport; Quantum-dot arrays; Renormalization methods; Fibonacci lattice

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1 Introduction

The study of electron transport in mesoscopic systems is a fundamental problem in nanophysics and nanotechnology [1,2] and rests on Landauer’s idea that conductance is proportional to phase-coherent electron transmittivity [3]. Within this context a great deal of attention has been given in recent years to electronic transport in a variety of structures including polymeric and molecular wires, nanotubes and quantum wires, quantum dots, and arrays and networks of quantum dots.

A semiconductor quantum dot (QD) is often described as an artificial atom, in which an external potential replaces the attractive potential of the nucleus to confine charge carriers in all three spatial directions [4,5]. The dot size is of the order of the Fermi wavelength in the host material, typically between 10 nm and 1 µm, and the confinement is usually achieved by electrical gating of a two-dimensional electron gas, often in combinations with etching of the material. Precise control of the number of electrons in the conduction band of a QD has been achieved in GaAs heterostructures [6]. An all-electrically controlled quantum dot array (QDA) can be realized by electrodes confining single electrons to the dot regions, with the electron tunnel between neighboring dots being controlled by electrical gating [7].

As in the case of real clusters, electronic transport through QDA’s can be treated theoretically within a tight-binding framework [8]. The tight-binding model has been used to study Coulomb effects on QD transmittance [9], magnetoconductance in chaotic arrays [10], Kondo resonances and Fano antiresonances in transport [11], and transport through two-dimensional networks [12,13,14]. A simplifying assumption treats a QD as a potential well, thus omitting a detailed account of its internal structure. This allows analytical results to be obtained for transport properties of QDA’s (see for instance [15,16]).

In this work we use the simple tight-binding approach to derive an analytical treatment of phase-coherent transport through a QDA model composed of two different sets of QD’s, as originally proposed by Mardaani and Esfarjani [15]. We treat both a periodic and quasi-periodic arrangement of the two types of QD’s in the array, and report comparative numerical illustrations of the density-of-states (DOS) and of the transmittivity of these arrays for a number $N$ of QD’s up to 100. Our analytical results allow us to evaluate very long arrays without any special numerical effort. Specifically, we use a decimation-renormalization method [17,18] to reduce the QDA to an effective dimer with renormalized site energies and hopping interactions, and supplement the method with a generalized Kirkman-Pendry relation [19,20] to account for the connection of the QDA to external metallic leads. The $T$-matrix
Formalism introduced in this paper for the calculation of the QDA transmittivity is equivalent to the formalism given in Ref. [21] for out-of-equilibrium leads in the special case of an infinitesimal bias and is suitable to deal with renormalized effective Hamiltonians describing very long chains.

2 Hamiltonian and density-of-states

We use a one-dimensional (1D) tight-binding Hamiltonian to describe a QDA of \( N \) equally spaced potential wells. The Hamiltonian can be written as

\[
H_{QD} = \sum_{i=1}^{N} \left\{ e_i |i\rangle \langle i| + (t_{i,i+1} |i\rangle \langle i+1| + t_{i+1,i} |i+1\rangle \langle i|) \right\},
\]

where the site energy \( e_i \) corresponds to the energy level for an electron in the \( i \)-th well and \( t_{i,i+1} = t_{i+1,i} \) is the hopping energy between the \( i \)-th and the \((i+1)\)-th well. The connection to external leads will be added later.

We focus on two types of QDA’s. The first is a periodic array in which two different types of QD’s, \( A \) and \( B \) say, alternate. In the second the two kinds of QD’s are arranged according to the Fibonacci sequence, i.e., if we define the first QD as \( F_1 = A \) and the second as \( F_2 = B \), the rest of the chain is built by the rule \( F_n = F_{n-1} F_{n-2} \). The schematic Hamiltonians for these QDA’s are shown in Fig. 1.

The related Green’s function at energy \( E \) is

\[
G(E) = \frac{1}{E - H_{QD}}.
\]

Here and below, we consider a complex energy variable defined as \( E + i\eta \) in the limit of vanishing positive imaginary part. To evaluate the DOS \( D(E) \) we use the Kirkman-Pendry relation [19], which relates the DOS to the matrix

Fig. 1. Schematic Hamiltonian for (a) a periodic QDA and (b) a Fibonacci QDA, for the case \( N = 12 \).
element $G_{1,N}(E)$ expressing coherence between the first and the last site of the QDA,

$$D(E) = \frac{1}{\pi} \text{Im} \frac{\partial}{\partial E} \ln G_{1,N}(E). \quad (3)$$

The matrix element $G_{1,N}(E)$ can be evaluated by reducing the QDA to an effective dimer through decimation of the intermediate QD’s (see for instance [17,18]). The renormalized array contains just the first and the last site and its Hamiltonian is expressed as a $2 \times 2$ matrix,

$$\tilde{H}_{\text{QD}}(E) = \begin{pmatrix} \tilde{\varepsilon}^{(N-2)}_1(E) & \tilde{t}_{1,N}(E) \\ \tilde{t}_{N,1}(E) & \tilde{\varepsilon}^{(N-2)}_N(E) \end{pmatrix}. \quad (4)$$

Here, the effective site and hopping energies can be obtained by the recursive relations

$$\tilde{\varepsilon}^{(j)}_1(E) = \tilde{\varepsilon}^{(j-1)}_1(E) + \tilde{t}_{1,j+1}(E) \frac{1}{E - \tilde{\varepsilon}^{(j-1)}_{j+1}(E)} t_{j+1,j+2}, \quad (5)$$

$$\tilde{\varepsilon}^{(j)}_{j+2}(E) = e_{j+2} + t_{j+2,j+1} \frac{1}{E - \tilde{\varepsilon}^{(j-1)}_{j+1}(E)} \tilde{t}_{j+1,1}(E), \quad (6)$$

$$\tilde{t}_{1,j+2}(E) = \tilde{t}_{1,j+1}(E) \frac{1}{E - \tilde{\varepsilon}^{(j-1)}_{j+1}(E)} t_{j+1,j+2} \quad (7)$$

and $\tilde{t}_{j+1,1} = \tilde{t}_{1,j+1}$ for $j \geq 1$, the initial values being given by the Hamiltonian parameters namely $\tilde{\varepsilon}^{(0)}_i(E) = e_i$ and $\tilde{t}_{1,2}(E) = t_{1,2}$. By direct inversion of $(E - \tilde{H}_{\text{QD}}(E))$ we obtain

$$G_{1,N}(E) = \frac{\tilde{t}_{N,1}(E)}{(E - \tilde{\varepsilon}^{(N-2)}_1(E))[E - \tilde{\varepsilon}^{(N-2)}_N(E)] - [\tilde{t}_{1,N}(E)]^2}. \quad (8)$$

We then use Eq. (3) to calculate the DOS.

In the illustrative calculations that we report here and in the following sections we have used the values of the parameters $e_A = -0.25$ eV, $e_B = 0.25$ eV, $t_{A,B} = 1.1$ eV and $t_{B,B} = 1.0$ eV. In Fig. 2 and Fig. 3 we show the DOS for QDA’s made from various numbers of QD’s in a periodic and a Fibonacci configuration. For small values of $N$ (see Fig. 2) the DOS shows $N$ peaks distributed over the energy range. For long chains with $N = 1000$ (see Fig. 3) the DOS is similar to that of an infinite array: in the periodic sequence (left panel in Fig. 3) there are two sub-bands separated by an energy gap of width...
Fig. 2. DOS of periodic array (left) and Fibonacci-ordered array (right) for the case $N = 4$ (solid line) and $N = 20$ (dotted line), as a function of energy $E$ referred to the center of the spectrum at energy $E_0$ and for a spectral width of $4t_0$.

Fig. 3. DOS as in Fig. 2, for the case $N = 1000$.

$|e_A - e_B|$, while in the case of a Fibonacci array (right panel in Fig. 3) the quasi-periodicity induces a fragmentation of the spectrum and the appearance of pseudo-gaps.

2.1 The effects of the leads

The QDA is next connected to an incoming $(l)$ and an outgoing $(r)$ metallic lead, which are described by two additional terms in the Hamiltonian,

$$H_{L,l} = \sum_{n=-\infty}^{1} \{E_0 |n\rangle\langle n| + t_0 (|n-1\rangle\langle n| + c.c.)\}$$

and

$$H_{L,r} = \sum_{n=N}^{\infty} \{E_0 |n\rangle\langle n| + t_0 (|n+1\rangle\langle n+1| + c.c.)\}.$$
Here the site energy $E_0$ in the leads and the hopping energy $t_0$ have been chosen equal to the center of the spectrum of the QDA and to one fourth of its spectral width. The presence of the leads modifies the DOS of the system and thus affects the electronic transport through the QDA. We accordingly have to decimate the leads and to consistently renormalize the energies of sites 1 and $N$ in the QDA.

Equation (3) does not apply in general and in particular, when sites 1 and $N$ in the array are not edge sites, a modified Kirkman-Pendry relation as derived by Farchioni et al. [20] must instead be used. This relation is

$$D(E) = \frac{1}{\pi} \text{Im} \left[ \frac{\partial}{\partial \lambda} \ln G_{1,N}(E, \lambda) \right]_{\lambda=0},$$

where the real parameter $\lambda$ is introduced to select the sites on which the electronic states are counted. In our specific case $G_{1,N}(E, \lambda)$ can be written as

$$G_{1,N}(E, \lambda) = \frac{\tilde{t}_{N,1}(\tilde{E})}{[\tilde{E} - \tilde{\varepsilon}_1^{(N-2)}(\tilde{E}) - \tilde{E}(E)][\tilde{E} - \tilde{\varepsilon}_N^{(N-2)}(\tilde{E}) - \tilde{E}(E)] - [\tilde{t}_{1,N}(\tilde{E})]^2},$$

where $\tilde{E} = E + \lambda$ and the term $\tilde{E}(E) = \frac{1}{2}(E - E_0) - \frac{1}{4}(E - E_0)^2 - t_0^2)^{1/2}$ is the renormalized contribution of the leads to the energy of sites 1 and $N$.

The DOS of a periodic QDA connected to an incoming and an outgoing lead is shown in Fig. 4. For small numbers of QD’s ($N = 4$ and $N = 12$) the effect of the leads is dominant and the DOS resembles that of a 1D monatomic lattice. A depression appears at the center of the spectrum for $N = 20$, and for a long array ($N = 100$) the effect of the leads becomes irrelevant and the DOS is very similar to that shown in the left panel of Fig. 3 for the isolated QDA. Similar effects on the DOS of the Fibonacci-ordered QDA are seen in Fig. 5: at low $N$ the peak structure shown in Fig. 2 is washed out by the presence of the leads, while at large $N$ the typical features due to quasi-periodicity appear.

At half filling the Fermi level is located near $(E - E_0)/t_0 = 0$ for all configurations, as is indicated in Figs. 4 and 5 by an arrow. In this case the DOS at the Fermi level vanishes on increasing the length of the periodic QDA. In a Fibonacci-ordered array, instead, the number of states at the Fermi level remains finite.
Fig. 4. DOS of periodic QDA connected to an incoming and an outgoing lead, as a function of energy $E$ referred to the band center at energy $E_0$ and for a bandwidth of $4t_0$. Left panel: $N = 4$ (solid line), $N = 12$ (solid line and dots) and $N = 20$ (dashed line). Right panel: $N = 100$.

Fig. 5. DOS as in Fig. 4, for a Fibonacci-ordered QDA connected to an incoming and an outgoing lead.

3 Transmission through the array

We rewrite the Hamiltonian $H = \tilde{H}_{\text{QD}} + H_{\text{L},l} + H_{\text{L},r}$ of the effective dimer representing the QDA connected to the leads as the sum of two terms, $H = H_0 + H_I$. The first term $H_0$ describes an infinite perfect chain with spacing $a$, site energy $E_0$ and hopping energy $t_0$, whose elements $(2, 3, \ldots, N - 1)$ have been decimated as previously described, and is given by

$$H_0 = H_{\text{L},l} + H_{\text{L},r} + (\tilde{E}_0 - E_0) \left(|1\rangle\langle1| + (|N\rangle\langle N|) + \tilde{t}_0(|1\rangle\langle N| + |N\rangle\langle 1|)\right). (13)$$

The remainder

$$H_I = \tilde{H}_{\text{QD}} - \{ \tilde{E}_0(|1\rangle\langle1| + (|N\rangle\langle N|) + \tilde{t}_0(|1\rangle\langle N| + |N\rangle\langle 1|)\} . (14)$$
will be viewed as a “perturbation” determining scattering of incoming waves. In these equations the quantities $\tilde{E}_0$ and $\tilde{t}_0$ are obtained from Eqs. (5) and (7) for $j = N - 2$ by taking $e_i = E_0$ and $t_i, i+1 = t_0$ for all $i$.

The wavefunction $|\varphi\rangle$ at energy $E$ in the continuous spectrum of $H$ is obtained from the wavefunction $|k\rangle$ of the unperturbed periodic Hamiltonian $H_0$, the unperturbed Green’s function $G^0(E) = (E - H_0)^{-1}$, and the $T$ matrix $T(E) = H_I(1 - G^0H_I)^{-1}$ as

$$|\varphi\rangle = |k\rangle + G^0 T |k\rangle,$$  

(15)

$T$ as well as $H_I$ being $2 \times 2$ matrices in the space spanned by $|0\rangle$ and $|N\rangle$. The projection of $|\varphi\rangle$ onto the localized function $|n\rangle$ is

$$\langle n|\varphi\rangle = \langle n|k\rangle + \sum_{l,m=0,1} G^0_{n,l} T_{l,m} \langle m|k\rangle,$$  

(16)

where $G^0_{n,l} = \langle n|G^0|l\rangle$, $T_{l,m} = \langle l|T|m\rangle$, and $\langle m|k\rangle = e^{ikna}$. The expressions for these matrix elements are given in [18]. We can then write Eq. (16) in the form

$$\langle n|\varphi\rangle = e^{ikna} + \left( G^0_{N,1} T_{1,N} + G^0_{1,N} T_{N,1} e^{-2i(N-1)a} + G^0_{N,N} T_{N,N} + G^0_{1,1} T_{1,1} \right) e^{ikna},$$

(17)

and define the transmittance $\tau$ and the reflectance $\rho$ by writing

$$\langle n|\varphi\rangle = \begin{cases} \tau e^{ikna} & (n > 1) \\ e^{ikna} + \rho e^{-ikna} & (n < 0) \end{cases}.$$  

We thus obtain

$$\tau = 1 + G^0_{N,1} T_{1,N} + G^0_{1,N} T_{N,1} e^{-2i(N-1)a} + G^0_{N,N} T_{N,N} + G^0_{1,1} T_{1,1}.$$  

(18)

Notice the difference between this Eq. (18), which is valid for both real and effective dimers, and Eq. (8) in Ref. [18] applies only to real dimers.

The transmission coefficient $T$ is given by $T = |\tau|^2$. Numerical results for the periodic and the Fibonacci-ordered QDA are shown in Figs. 6 and 7. The features of the transmittivity as a function of the energy parallel those of the DOS in Figs. 4 and 5, where the effects of the leads have been included: the transmittivity drops as the DOS decreases and vanishes in the energy gaps. At half filling in the periodic array the transmittivity at the Fermi level is high for very short arrays but rapidly drops on increasing the number of dots,
Fig. 6. Transmittivity coefficient for a periodic QDA as a function of the energy $E$, referred to the band center at energy $E_0$ and for a bandwidth of $4t_0$. Left panel: $N = 4$ (solid line), $N = 12$ (solid line and dots) and $N = 20$ (dashed line). Right panel: $N = 100$.

Fig. 7. Transmittivity coefficient as in Fig. 6, for a Fibonacci-ordered array.

so that the array becomes insulating. On the contrary, in a Fibonacci-ordered array the transmittivity near the Fermi level remains high, so that metallic-like conduction is preserved independently of the length of the array. There are, however, strong minima in the transmittivity in correspondence to the pseudo-gaps in the DOS.

4 Concluding remarks

In summary, we have presented a fully analytical method for the calculation of the density of electron states and the phase-coherent electron transport coefficient in a linear array made of an arbitrary number of two different types of potential well with different energy levels. We have specifically considered both a periodic sequence of pairs of potential wells and a sequence in which the two types of potential wells are arranged according to the Fibonacci se-
quence. In both cases the connection of the array to external metallic wires has been included. The method does not explicitly diagonalize the tight-binding Hamiltonian of the system, but uses a decimation-renormalization procedure to reduce the array to an effective dimer, which is then treated by a suitably adapted $T$-matrix scattering approach.

The density of states and the transmittivity vanish at the same energy when the connection to external metallic wires is included. The calculations explicitly show that an energy gap opens in the periodic array as its length is increased, so that metallic conductance turns into insulating behavior in the case of single occupancy of each well. With increasing length the Fibonacci-ordered array develops instead pseudo-gaps away from the band center, and again a metal-to-insulator transition is expected for appropriate values of the filling factor.

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