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Correlation between the phase of transmission resonances and parity of bound states in a quantum dot

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Abstract. We investigate the phase of the transmission peaks of electrons in a single-channel system with a quantum dot embedded between the leads. The quantum dot is modelled by a tight-binding Hamiltonian of a cluster of a two- or three-dimensional lattice which is connected with one-dimensional leads. We derive an exact expression which relates the transmission amplitude to the bound states of the dot. It is confirmed that the abrupt phase changes in the transmission amplitude are associated with the transmission peaks and zeros. The phase at the resonance peaks is related to the parity of the corresponding bound states of the dot. On the basis of the exact expression a possible explanation of the in-phase features discovered in the experiments is presented.

1. Introduction

The transport properties of electronic devices are usually characterized on the basis of conductance measurements which explore the relationship between the current and the applied bias voltage. However, for mesoscopic systems, such as quantum dots [1, 2], whose size is comparable with the wavelength of the wavefunctions of the electrons, the magnitude of the conductance is not sufficient for describing the transport properties because the wave nature of the electrons plays an important role in this case [3, 4]. In 1995, Yacoby *et al* reported the first measurement of the phase change of electrons in transmission through a quantum dot by using the interference in an Aharonov–Bohm (AB) ring threaded with a magnetic flux [3]. The quantum dot is embedded in an arm of the AB ring and the phase of electrons transmitted through the dot is determined from the relative phase of the AB oscillation. In the experiment two main features were observed: the AB oscillations have the same phase at the successive conductance peaks, and the phase changes abruptly by π when the dot potential scans through a single resonance peak. Since then, great efforts have been made to explain these features [5–9]. Further experimental investigations revealed more details about the phase of the electron transport through a dot [4, 10]. Theoretically, it has been shown that there should be a phase change of π for every conductance peak, but another feature—that the consecutive peaks are in phase—is not well understood yet [4]. In reference [9] the transmission properties of electrons were investigated by the use of the one-dimensional (1D) non-interacting model, and the in-phase feature observed in the experiments was attributed to the effect of interference between two AB arms. Another theory based on the Friedel sum rule

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was presented in reference [11]. This theory tries to find a solution of the problem from a new viewpoint. One of the observations is that the 1D Friedel sum rule

$$\Delta Q/e = \Delta \arg(t)/\pi \tag{1}$$

(where Q is the charge tunnelling through the dot and t is the transmission amplitude) is not strictly valid for quasi-1D systems due to the appearance of the transmission zeros. One immediate consequence is that there are two possibilities for adjacent resonances. They can be either out of phase by π or in phase, and in the latter case a transmission zero occurs in between. The theory also studies how the wavefunction nodes of the quasibound states of the dot affect the phase of the transmission amplitude. It predicts that the 'spanning' nodes which connect two opposite boundaries of the dot shift the phase by π, while the 'non-spanning' nodes which touch either only one boundary or no boundary at all do not alter the phase. This theory demonstrates that both in-phase and out-of-phase-by-π features for the consecutive resonances are possible, but it cannot explain the in-phase behaviour of a long series of resonances observed in the experiments.

In this paper we present a rigorous expression which relates the amplitude of transmission of electrons through the dot and the wavefunctions of the bound states. In the derivation the leads are modelled with a 1D tight-binding Hamiltonian but the dot is represented by a 2D or 3D cluster with any shape. It is found that the phase of the transmission amplitude is closely related to the symmetry of the bound states of the dot and the coupling between the leads and the dot. The out-of-phase resonance peaks are suppressed if the dot is small enough and the coupling between the leads and the dot has a long-range feature in comparison with the dot size. This results in in-phase behaviour for the consecutive peaks in a long series and provides a possible explanation of the experiments.

The paper is organized as follows: in the next section the model used to investigate the tunnelling through the dot is described; in the third section the expression for the transmission amplitude is derived; in the fourth section the calculated results for 2D and 3D dots with different shapes are presented; the last section is devoted to a brief summary of the conclusions.

2. The model

We study a tight-binding model of a quantum dot embedded between two leads. The leads are represented by 1D chains while the dot is a 2D or 3D cluster with arbitrary shape. The Hamiltonian can be written as

$$\mathcal{H} = \mathcal{H}_d + \mathcal{H}_l + \mathcal{H}_c \tag{2}$$

where $\mathcal{H}_d$, $\mathcal{H}_l$, and $\mathcal{H}_c$ are the sub-Hamiltonians for the dot, the leads, and the coupling between them, respectively. In a tight-binding scheme they can be written as

$$\mathcal{H}_d = \sum_{i\in\mathcal{D}} (V + \epsilon_i) d_i^\dagger d_i - t_d \sum_{\langle ij\rangle\in\mathcal{D}} d_i^\dagger d_j \tag{3}$$

$$\mathcal{H}_l = -t_0 \sum_{m\neq -1,0} (c_m^\dagger c_{m+1} + \text{H.c.}) \tag{4}$$

$$\mathcal{H}_c = -\sum_{i\in\mathcal{D}} (t_{-1,i} c_{-1}^\dagger d_i + t_{1,i} c_1^\dagger d_i + \text{H.c.}) \tag{5}$$

where c_m and d_i are annihilation operators of electrons at the mth site of the leads and at the ith site of the dot, t_0 and t_d are nearest-neighbour hoppings in the leads and the dot, respectively, $t_{-1,i}$ and $t_{1,i}$ are the couplings between the contact points in the leads ($m = -1, 1$) and the sites on the dot, ϵ_i is the site energy at the ith site of the dot, V is the dot potential induced by the gate voltage. Here m is the 1D coordinate of the sites in the leads, and the dot is at coordinate $m = 0$. $\mathcal{D}$ denotes the set of sites of the dot. Owing to the small size of the dot, the couplings between the contact points of leads and all the sites of the dot are taken into account. The transmission of electrons through the dot is strongly dependent on the dot bound states and the couplings between leads and dot.

In the experiments of Yacoby *et al* [3] the dot is embedded in one arm of an AB ring through which a magnetic flux is applied to measure the phase difference between the two arms caused by the dot. In this case the sub-Hamiltonian $\mathcal{H}_l$ is changed to

$$\mathcal{H}_l = -t_0\left[\left(\sum_{m=-L+1}^{-2} + \sum_{m=1}^{L-2}\right)c_m^\dagger c_{m+1} + \sum_{m=-L+1}^{L-2} c_{1,m}^\dagger c_{1,m+1} + \left(\sum_{m=-\infty}^{-L-1} + \sum_{m=L}^{\infty}\right)c_{0,m}^\dagger c_{0,m+1} + \text{H.c.}\right]$$
$$- t_0(c_{0,-L}^\dagger c_{-L+1} + c_{0,-L}^\dagger c_{1,-L+1} + c_{L-1}^\dagger c_{0,L} + c_{1,L-1}^\dagger c_{0,L} + \text{H.c.}) \quad (6)$$

and the hopping integral $t_{-1,i}$ in equation (5) is changed to $t_{-1,i}\exp(\mathrm{i}\phi)$, where $c_{0,m}$ and $c_{1,m}$ are annihilation operators of electrons at the mth site outside the AB ring and in the arm without the dot of the ring, respectively, $2L$ is the length of one arm, and ϕ is the flux through the ring. Here we use a gauge where the phase of hopping integrals caused by the flux appears only in an extremal bond connected to the dot.

3. The formula for the transmission amplitude

The flux dependence of the transmission through the AB ring with a dot embedded in an arm is governed by the quantum interference of the two arms where the phase difference caused by the dot plays a dominant role. At first, we calculate the transmission and reflection amplitudes of electrons at the dot embedded in a single chain. From these results we can calculate the transmission through the AB ring. In the one-chain Hamiltonian equation (2), sub-Hamiltonian $\mathcal{H}_d$ can be diagonalized to obtain the energy levels $\{E_j\}$ and the wavefunctions $\{\phi_j\}$ of the bound states of dot. ϕ_j can be expressed as a linear combination of the site states:

$$\phi_j = \sum_{i\in\mathcal{D}} b_{ji} d_i^\dagger |0\rangle \quad (7)$$

with $|0\rangle$ being the vacuum. On the basis of these states, the one-chain Hamiltonian can be rewritten as

$$\mathcal{H} = \mathcal{H}_l + \sum_j [E_j a_j^\dagger a_j - (t_j^L c_{-1}^\dagger a_j + t_j^R c_1^\dagger a_j + \text{H.c.})] \quad (8)$$

where a_j is the annihilation operator of electron in state ϕ_j, and

$$t_j^{L(R)} = \sum_{i\in\mathcal{D}} b_{ji} t_{-1\,(1),i}. \quad (9)$$

We consider that a plane wave is incident from the left-hand lead. In this case the wavefunction of the tunnelling electron is

$$\psi = \sum_{m\leqslant -1} (\mathrm{e}^{\mathrm{i}k(m+1)} + r\mathrm{e}^{-\mathrm{i}k(m+1)})c_m^\dagger|0\rangle + \sum_{m\geqslant 1} t\mathrm{e}^{\mathrm{i}k(m-1)}c_m^\dagger|0\rangle + \sum_j \xi_j a_j^\dagger|0\rangle \quad (10)$$

where t and r are the amplitudes of transmitted and reflected waves, respectively, ξ_j is the amplitude in the jth bound state of the dot, and k is the wave vector of the incident wave satisfying $E = -2t_0\cos k$ with E being the energy. By applying Hamiltonian (8) to this wavefunction, one obtains the following equations for t, r, and ξ_j:

$$E\xi_j = E_j\xi_j - t_j^{L*}(1+r) - t_j^{R*}t \qquad \text{for all } j \quad (11)$$

$$E(1+r) = -t_0(\mathrm{e}^{-\mathrm{i}k} + r\mathrm{e}^{\mathrm{i}k}) - \sum_j t_j^L \xi_j \tag{12}$$

$$Et = -t_0\mathrm{e}^{\mathrm{i}k} - \sum_j t_j^R \xi_j. \tag{13}$$

By solving these equations we obtain the transmission and reflection amplitudes:

$$t = \frac{2\mathrm{i}t_0 Q_{LR}\sin k}{[t_0\exp(-\mathrm{i}k) + Q_{RR}][t_0\exp(-\mathrm{i}k) + Q_{LL}] - |Q_{LR}|^2} \tag{14}$$

$$r = -\frac{2\mathrm{i}t_0[Q_{RR} + t_0\exp(-\mathrm{i}k)]\sin k}{[t_0\exp(-\mathrm{i}k) + Q_{RR}][t_0\exp(-\mathrm{i}k) + Q_{LL}] - |Q_{LR}|^2} - 1 \tag{15}$$

where

$$Q_{\lambda\lambda'} = \sum_j \frac{t_j^{\lambda *} t_j^{\lambda'}}{E - E_j}.$$

It can be seen that at the resonances ($E = E_j$) the transmission amplitude is

$$t(E)\big|_{E=E_j} = 2\mathrm{i}t_0 t_j^R t_j^{L*}\sin k \bigg/ \left(t_0\mathrm{e}^{-\mathrm{i}k}(|t_j^L|^2 + |t_j^R|^2) + \sum_{j'\neq j} \frac{|t_{j'}^L t_j^R - t_{j'}^R t_j^L|^2}{E_j - E_{j'}} \right). \tag{16}$$

At the weak-coupling limit, $|t_j^R t_j^L| \ll |t_0(E_j - E_{j'})|$, one has

$$t(E)\big|_{E=E_j} \sim \frac{2\mathrm{i}t_j^R t_j^{L*}\sin k}{\mathrm{e}^{-\mathrm{i}k}(|t_j^L|^2 + |t_j^R|^2)}. \tag{17}$$

This means that in this case the intensity of the resonance peaks is only dependent on the lead–dot coupling. On the other hand, if the level spacing is small compared with $|t_j^R t_j^L/t_0|$, the intensity of the peaks is influenced by the nearby resonance levels. In particular, if the bound states of two adjacent levels E_j and $E_{j'}$ have opposite (or near opposite) parity, with the result that $|t_{j'}^L t_j^R - t_{j'}^R t_j^L| \gg |(E_j - E_{j'})t_0|$, then the corresponding transmission peaks will be drastically suppressed. In spite of the different peak values at the resonances, the transmission amplitude changes sign when sweeping through a resonance, leading to an abrupt jump of phase by π.

If $\mathcal{H}_d$ is a real symmetric matrix, t_j^R and t_j^L are also real. If $t_j^R t_j^L$ and $t_{j'}^R t_{j'}^L$ have the same sign for two adjacent levels E_j and $E_{j'}$, Q_{LR} changes sign when E sweeps from E_j to $E_{j'}$. This results in a transmission zero in between. This is the same as the conclusion derived from the Friedel sum rule [11], but now it is expressed with an analytic formula. Since the transmission amplitude changes sign at the transmission zero, the phase will also jump by π at that point, leading to the in-phase feature of the resonance peaks at adjacent resonances E_j and $E_{j'}$. On the other hand, there is no transmission zero in between if $t_j^R t_j^L$ and $t_{j'}^R t_{j'}^L$ have opposite signs, leading to an out-of-phase feature for adjacent levels E_j and $E_{j'}$.

Now we come to the conclusion that the in-phase feature for two adjacent levels occurs only if $t_j^R t_j^L$ has the same sign for them. If the in-phase feature appears in a long series of the resonances, the only reasonable explanation is that $t_j^R t_j^L$ has the same sign for all of them. However, this could not be satisfied by the bound states of a dot. In fact, if the dot is modelled by a 1D chain, $t_j^R t_j^L$ will change sign alternately when varying the energy. A possible solution for this is that the peaks of different sign of $t_j^R t_j^L$ are effectively suppressed. This is indeed the case if the dot is small enough and the hoppings between the contact points of the leads and the sites of the dot are of long range compared with the size. In particular, if

$$t_{-1,i} = t_{1,i} = t' \qquad \text{for all } i \in \mathcal{D} \tag{18}$$

and the system has reflection symmetry about the centre of the dot, a bound state, ϕ_j, has odd or even parity and the $t_j^{L(R)}$ in equation (9) are non-zero only for ϕ_j with even parity. In this case all the out-of-phase peaks are completely suppressed. In the next section we will present calculated results for transmission amplitudes for several 2D and 3D samples with more general parameters.

From the t and r obtained for the dot, one can calculate the gross transmission of the AB ring. We denote the chain segments of the left lead, right lead, arm of ring without dot, left branch of arm with dot, and right branch of arm with dot as S_1, S_2, S_3, S_4, and S_5, respectively. Since they are uniform chain segments, the coefficients of the wavefunction for them are described with amplitudes of forward and backward plane waves A_j and B_j, with j from 1 to 5. From the Hamiltonian one has equations for them:

$$A_5 = A_4/t^* - r^* B_4/t^* \qquad B_5 = -r A_4/t + B_4/t \tag{19}$$

$$A_4 \mathrm{e}^{-\mathrm{i}k(L-1)} + B_4 \mathrm{e}^{\mathrm{i}k(L-1)} = A_3 + B_3 = A_1 + B_1 \tag{20}$$

$$A_5 \mathrm{e}^{\mathrm{i}k(L-1)} + B_5 \mathrm{e}^{-\mathrm{i}k(L-1)} = A_3 \mathrm{e}^{2\mathrm{i}kL} + B_3 \mathrm{e}^{-2\mathrm{i}kL} = A_2 + B_2 \tag{21}$$

$$E(A_1 + B_1) = -t_0(A_1 \mathrm{e}^{-\mathrm{i}k} + B_1 \mathrm{e}^{\mathrm{i}k} + A_3 \mathrm{e}^{\mathrm{i}k} + B_3 \mathrm{e}^{-\mathrm{i}k} + A_4 \mathrm{e}^{-\mathrm{i}k(L-2)} + B_4 \mathrm{e}^{\mathrm{i}k(L-2)}) \tag{22}$$

$$E(A_2 + B_2) = -t_0(A_2 \mathrm{e}^{\mathrm{i}k} + B_2 \mathrm{e}^{-\mathrm{i}k} + A_3 \mathrm{e}^{\mathrm{i}k(2L-1)} + B_3 \mathrm{e}^{-\mathrm{i}k(2L-1)} + A_5 \mathrm{e}^{\mathrm{i}k(L-2)} + B_5 \mathrm{e}^{-\mathrm{i}k(L-2)}). \tag{23}$$

By setting $A_1 = 1$, $B_2 = 0$, $B_1 = r_g$, and $A_2 = t_g$, we can solve from these equations the gross transmission amplitude t_g. Note that in the presence of the magnetic flux, t_j^L in equation (9) becomes $t_j^L \mathrm{e}^{\mathrm{i}\phi}$. At the resonance of the tunnelling of the dot, $|t| \sim 1$ and $r \sim 0$, so one has $t \sim \mathrm{e}^{\mathrm{i}\phi_0 - \mathrm{i}\phi}$ where ϕ_0 is the phase shift produced by the dot in the absence of flux. By tuning the flux ϕ, the phase shift ϕ_0 can be compensated to get a constructive interference in the AB ring. In this way one can get information on the dot phase shift ϕ_0 by measuring the compensating flux at the resonances.

4. Calculated transmission amplitudes of 2D and 3D samples

For a dot of any shape and potential profile, $\mathcal{H}_d$ can be numerically diagonalized. From the eigenvalues and eigenfunctions obtained one can calculate the transmission amplitude from equation (14).

First we consider a 2D round dot with radius R_0. The hoppings between the leads and the dot are described by equation (18). In figure 1 we plot the calculated magnitude ($|t|^2$) and the phase ($\arg(t)$) of the transmission amplitude. It can be seen that in this case all of the out-of-phase peaks are completely suppressed. The phase changes by π at the peaks and all the peaks have the same phase. The same calculations are done for a 3D sphere dot and the results are shown in figure 2. The hoppings between the leads and the dot are still of the form of equation (18). It can be seen that in this case the in-plane feature of the resonances remains. The peaks are denser in the 3D case due to the increase of the number of dot states.

Secondly we consider the case where the hoppings between the lead contact points and the sites of dots are exponentially decreased with increasing distance:

$$t_{m,i} = t'' \exp(-r_{m,i}/r_0) \qquad \text{for } m = -1, 1 \tag{24}$$

where $r_{m,i}$ is the distance between contact point m and dot site i, and r_0 is the damping length. The transmission coefficient and the phase calculated from equation (24) for a 2D round dot and a 3D spherical dot are shown in figures 3 and 4, respectively. It can be seen that in this

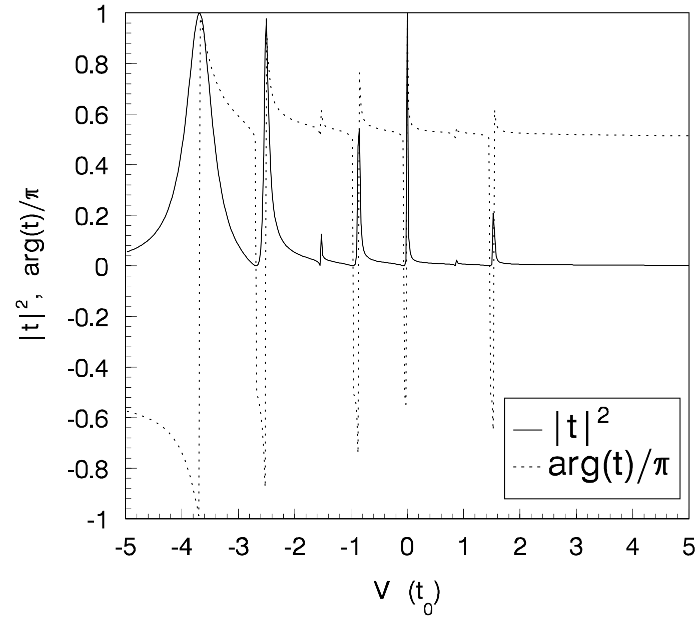

Figure 1. The transmission coefficient $|t|^2$ and the phase of the transmission amplitude $\arg(t)$ as functions of the dot potential V for a 2D round dot with radius $R_0 = 4$ lattice spacing. The couplings between the leads and the dot are described by equation (18) with $t' = 0.06t_0$. The other parameters are $E = 0$, $t_d = t_0$.

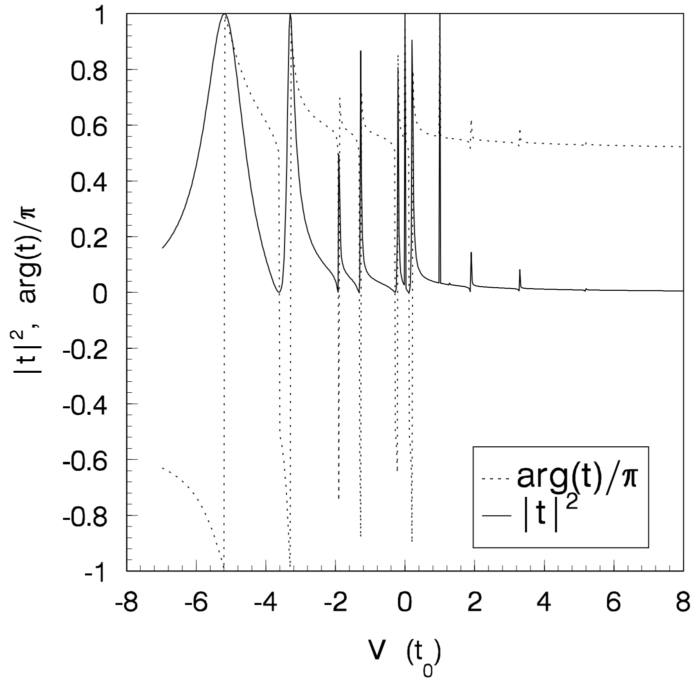

Figure 2. $|t|^2$ and $\arg(t)$ as functions of the dot potential V for a 3D spherical dot with radius $R_0 = 3$ lattice spacing. The other parameters are the same as for figure 1.

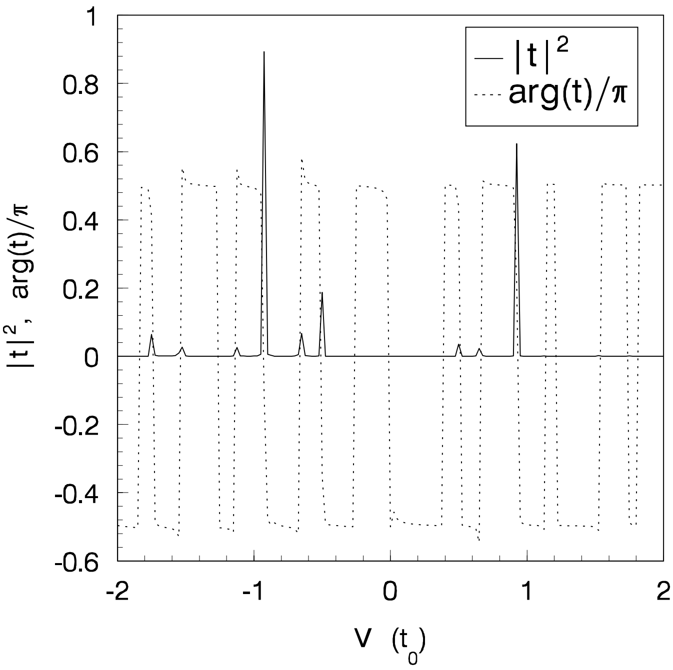

Figure 3. $|t|^2$ and $\arg(t)$ as functions of the dot potential V for a 2D round dot with radius $R_0 = 4$ lattice spacing. The couplings between the leads and the dot are described by equation (24) with $t'' = 0.12t_0$ and $r_0 = 3$ as the lattice spacing. The other parameters are the same as for figure 1.

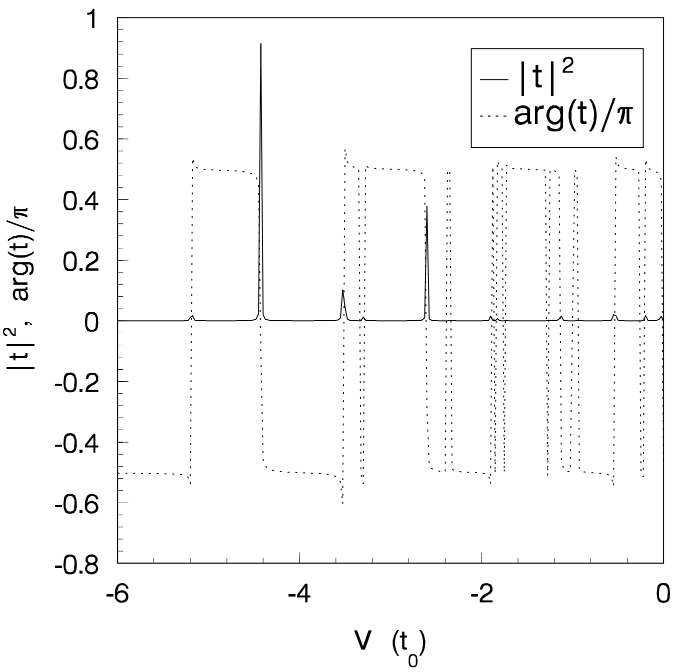

Figure 4. $|t|^2$ and $\arg(t)$ as functions of the dot potential V for a 3D spherical dot with radius $R_0 = 3$ lattice spacing. The other parameters are the same as for figure 3.

case the phase jumps at the peaks more abruptly; out-of-phase peaks appear, but they are still remarkably suppressed compared with the in-phase peaks.

Now we consider the case where the reflection symmetry is broken. This is realized by introducing site-energy fluctuations in the dot. The calculated transmission coefficient and the phase calculated for the 2D round dot and 3D spherical dot are shown in figures 5 and 6, respectively. The hoppings between the leads and the dot are of the form of equation (18). We can see that in this case the peaks have almost the same phase. However, there appear slight fluctuations of the peak phase, reflecting the randomness of the site energy.

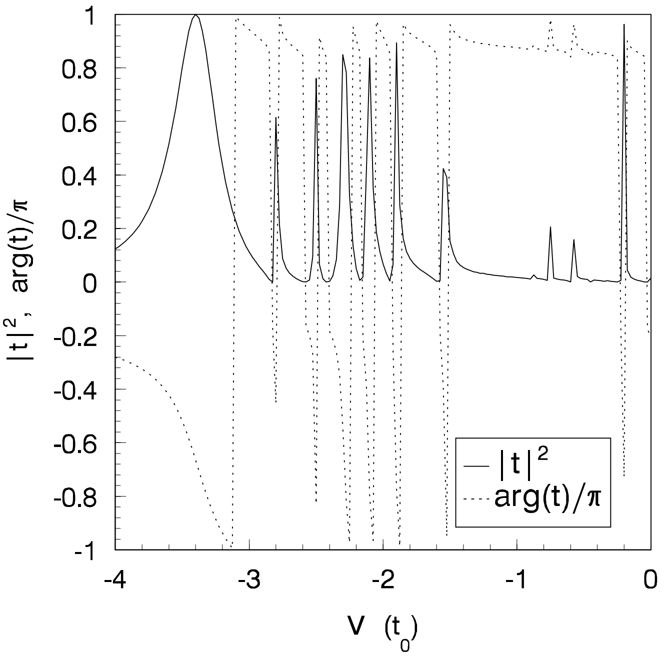

Figure 5. $|t|^2$ and $\arg(t)$ as functions of the dot potential V for a 2D round dot with radius $R_0 = 4$ lattice spacing. The couplings between the leads and the dot are described by equation (18) with $t' = 0.06t_0$. The site energies of dots are randomly distributed between $-0.5t_0$ and $0.5t_0$. The other parameters are the same as for figure 1.

At finite temperatures, the measurable quantity is the conductance through the AB ring, and information on the transmission phase shift of the dot is obtained from the compensating flux. From the Landauer formula one can calculate the conductance as

$$G(T) = -\frac{e^2}{h}\int \mathrm{d}E \sum_{\mathcal{O}} F_{\mathcal{O}}(T)\frac{\partial f(E,T)}{\partial E}|t_g^{(\mathcal{O})}(E)|^2 \tag{25}$$

where f is the Fermi distribution of free electrons in the leads:

$$f(E,T) = \frac{1}{1+\mathrm{e}^{(E-\mu)/(k_BT)}}.$$

Also, $F_{\mathcal{O}}(T)$ is the thermal probability of the dot state with occupied levels of set $\mathcal{O}$:

$$F_{\mathcal{O}}(T) = \prod_{j\in\mathcal{O}} \frac{1}{1+\mathrm{e}^{(E_j-\mu)/(k_BT)}} \tag{26}$$

where μ is the chemical potential, and $t_g^{(\mathcal{O})}(E)$ is the gross transmission amplitude of the ring calculated from the equations of the last section, but level index j in equations (11), (12), and

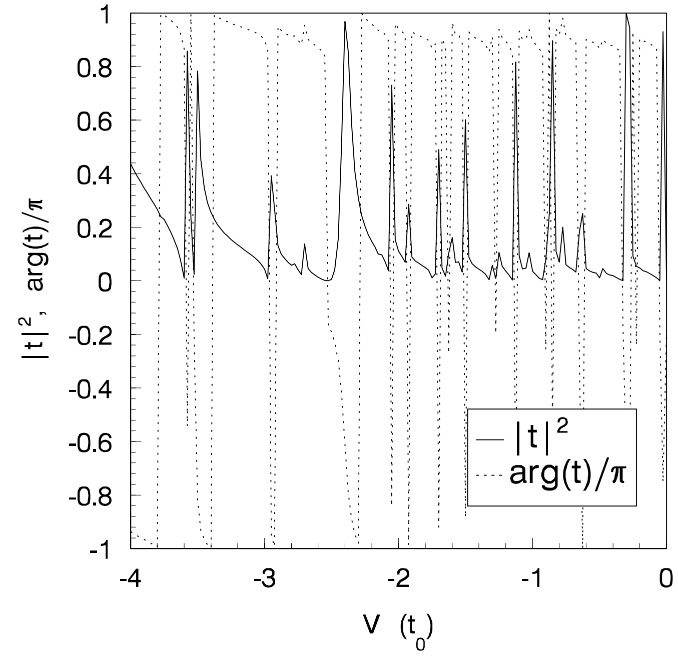

Figure 6. $|t|^2$ and $\arg(t)$ as functions of the dot potential V for a 3D spherical dot with radius $R_0 = 3$ lattice spacing. The other parameters are the same as for figure 5.

(13) is for the empty levels outside set $\mathcal{O}$. Here we omit the spin index. From the thermal distribution it can be seen that the behaviour of the transmission peaks and compensating flux is still described by the transmission amplitude t if $k_B T$ is much smaller than the level spacing. If the temperature is too high, the transmission resonances of the dot and the quantum interference of the ring will be destroyed by the thermal fluctuations.

5. Conclusions

From a tight-binding single-electron Hamiltonian we derive a rigorous expression which relates the amplitude of transmission of electrons through the dot and the wavefunctions of the bound states. In the derivation the leads are modelled with a 1D tight-binding Hamiltonian but the dot is represented by a 2D or 3D cluster with any shape. It is confirmed that the abrupt phase changes in the transmission amplitude are associated with the transmission peaks and zeros. The phase at the resonance peaks is related to the parity of the corresponding bound states of the dot. It is found that the out-of-phase resonance peaks are suppressed if the dot is small enough and the coupling between the leads and the dot has a long-range feature in comparison with the dot size. This results in the in-phase behaviour for the consecutive peaks in a long series and provides a possible explanation for the phenomena observed in experiments.

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