Coulomb effects on the transmittance of open quantum dots in a tight-binding model

A. Aldea, A. Manolescu, and V. Moldoveanu

National Institute of Materials Physics,
P. O. Box MG-7 Bucharest-Magurele, Romania

Abstract
A quantum-mechanical calculation of conductance in an open quantum dot is performed in the Landauer-Büttiker formalism using a tight binding Hamiltonian with direct Coulomb interaction. The charge distribution in the dot is calculated self-consistently as function of a gate potential, for various dot-leads couplings. The interaction is active only inside the dot, but not in the leads, its strength being an input parameter. Our calculations are complementary to the master-equation approach [1], go beyond the “orthodox theory”, and account for the size, tunneling, and interaction effects in quantum dots.

1 Introduction
It is known that the electron-electron interaction (EEI) is important in the transport properties of small systems such as quantum dots (QD’s). The standard approach is the so-called ”orthodox theory”, which neglects the size quantization and reduces the quantum mechanics to the charge quantization inside a capacitor [2]. In this paper we propose a pure quantum-mechanical method, based on the Landauer-Büttiker (LB) formalism and the Hartree approximation (HA). We consider a discrete, tight-binding model, which allows the tailoring of different shapes of the QD and the presence of a magnetic field in the Peierls’ fashion. The properties are controlled by several inputs: a) the coupling of the QD with external leads, $t_{LD}$; b) the size and shape of the dot which determines the electronic spectrum in the absence of the EEI; c) the interaction strength, $U$. The calculations are performed self-consistently in the HA for dots of rectangular shape with four attached leads, accommodating up to 40 electrons. The energy spectrum, transmittance, and dot charging are calculated and discussed.

2 The formalism
We model the quantum dot as a 2D rectangular plaquette weakly coupled to external leads. In the tight-binding picture the Hamiltonian consists of three.
terms, $H^D$ describing the isolated QD, $H^L$ for the leads, labeled by $\alpha$, and $H^{LD}$ for the coupling:

$$H = H^D + \sum_\alpha H^L_\alpha + \sum_\alpha H^{LD}_\alpha.$$  \hspace{1cm} (1)

Since the role of the leads is only to inject and drain the electrons, we neglect the EEI in $H^L$, and include it only in $H^D$. Meir and Wigreen and Gartner \cite{3} have shown, using different approaches, that in this situation the LB formalism remains valid.

In this approach the Fermi level $E_F$ is fixed by the infinite leads, and the external gate $V_g$ is simulated by the site energy in $H^D$:

$$H^D = \sum_i \left( V_g + U \sum_{j \neq i} \frac{\langle n_j \rangle}{|i-j|} \right) |i \rangle \langle i| + t_D \sum_{<i,i'>} |i \rangle \langle i'|.$$  \hspace{1cm} (2)

$\langle n_j \rangle$ is the mean occupation number of the site $j \in$ QD, and $U$ is the parameter describing the EEI. We choose $t_D = 1$ (i.e. the energy unit is the hopping integral in QD) and denote by $<i,i'>$ the nearest-neighbours summation. Instead of using the whole Hamiltonian (1), it is convenient to describe the open QD by an effective Hamiltonian with a non-hermitic term which depends on energy $E$ and incorporates the influence of the leads:

$$H^D_{\text{eff}} = H^D + H^{DL}(E - H^L)^{-1}H^{LD} = H^D + \tau^2 t_L \sum_\alpha e^{-ik} |\alpha \rangle \langle \alpha|,$$  \hspace{1cm} (3)

where $t_L$ is the hopping energy of leads, $\tau = t_{LD}/t_L$, $k$ is defined by $2t_L \cos k = E$, and $|\alpha\rangle$ stands for the dot state where the lead $\alpha$ is attached.

The matrix elements of the Green’s function $G^{-}_{jj}(E) = \langle j | (E - H_{\text{eff}} + i0)^{-1} | i \rangle$ are calculated numerically using Eqs.(2-3) and the self-consistency condition

$$\langle n_j \rangle = \frac{1}{\pi} \int_{-\infty}^{E_F} \text{Im} \ G^{-}_{jj}(E) \, dE.$$  \hspace{1cm} (4)

In the LB formalism the conductance matrix $g_{\alpha\beta}$ is given by the transmittance between the leads $\alpha$ and $\beta$:

$$g_{\alpha\beta} = \frac{e^2}{h} T_{\alpha\beta} = \frac{e^2}{h} \tau^4 t_L^2 \sin^2 k \ |G^+_{\alpha\beta}(E_F)|^2, \ \alpha \neq \beta.$$  \hspace{1cm} (5)

In the weak-coupling limit $\tau \ll 1$, the transport problem is reduced to a tunneling problem, and the transmittance shows resonances corresponding to the energy spectrum of the isolated QD with the many-body effects included. The position, width and heights of the peaks depend on the above mentioned parameters.

### 3 Results and discussion

Each transmittance peak corresponds to the addition of an extra electron in a Coulomb blockade mechanism (for a review see Ref. 2). The position and
width of resonances can be correlated to the Hartree spectrum of the isolated QD displayed in Fig.1 vs. $E_F$. The spectrum is independent of $E_F$ as long as the later is not sufficiently close to an energy level. When $E_F$ approaches the $n$-th eigenvalue of the system with $N$ electrons, and the addition of the $N+1$-th electron becomes possible, the whole spectrum raises with the additional energy $E_{\text{add}}(N, N+1) = E_n(N+1) - E_n(N)$. The essential characteristic is that the $E_{\text{add}}$ is not supplied step-like but it is gained linearly with increasing $E_F$ in an interval $\Delta E_F = E_{\text{add}}$ (in this region, a slope=1.0 is evident in Fig.1). This calculation shows that $E_{\text{add}}(N, N+1)$ depends on the number of electrons $N$ and on the interaction strength $U$. With increasing $U$, $E_{\text{add}}$ increases, the plateaus of the energy levels shrink, while those of the number of particles increase. A new electron is added exactly in the middle of the interval $\Delta E_F$, i.e. at $E_F = (E_n(N) + E_n(N+1))/2$, see the diagonal line of Fig.1. These charge-degeneracy points correspond to the resonance peaks in Fig.2b. The Coulomb blockade is accompanied by the so-called (elastic) cotunneling effect meaning that the transmittance is non-vanishing also in a range about the degeneracy point $\Theta$. This effect gives rise to some width of the Coulomb oscillations. The comparison of Fig.1 and Fig.2b shows that the width at the bottom of a conductance peak equals $E_{\text{add}}$, indicating that, for small $t_{LD}$, the cotunneling at resonance is of Coulomb origin. The number of electrons in the dot is a rather smooth function of the gate potential $V_g$, i.e. the steps of Fig.2a are not well defined even for a weak coupling (the dotted line), in spite of the fact that the transmittance shows sharp peaks. One notices that each of these peaks points to an ideal step of Fig.2b, which corresponds to the limit $\tau \to 0$. For $\tau \sim 0.3 - 0.5$, the tunneling effects become more important: the intra-valley cotunneling $\tilde{\delta}$ appears and even the resonance width is now determined by tunneling. With still increasing the dot-leads coupling the resonances are spoiled, the charge quantization is totally lost and, if a strong enough magnetic field is applied, typical quantum Hall effects appear. We mention that here $t_{LD}$ is present in all powers of the perturbation theory.

4 Conclusions

This approach based on Landauer-Büttiker formalism, tight-binding Hamiltonian and Hartree approximation is able to describe the interplay of the size, interaction, and tunneling in QD. Due to the size effects, the addition energy (in other words, the inverse of the dot capacitance) depends on the number of electrons, and the Coulomb oscillations of the conductance are distributed irregularly. Both intra-valley and at-resonance cotunneling can be put into evidence; at resonance, a competition between tunneling and interaction is present. Increasing the tunneling parameter, the charge quantization vanishes faster than the resolution of the Coulomb peaks of the conductivity; the peaks are enforced by the charge-degeneracy condition.
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Figure 1: The energy spectrum of the isolated QD vs. $E_F$, calculated self-consistently in the Hartree approximation for $U = 0.5$.

Figure 2: (a) The number of particles vs. the gate potential for $U = 0$ (the noninteracting system) and for $U = 0.5$. With solid lines - the limit $\tau \to 0$, with dashed lines - the weakly coupled system, $\tau = 0.1$. (b) The conductance $g_{12}$ in the tunneling regime, for $U = 0.5$, with solid line, with maxima corresponding to the steps in the number of particles. The dash-dotted line shows the conductance for $U = 1$. 