We study theoretically the appearance of quantum correlations in two- and three-electron scattering in single and double dots. The key role played by transport resonances into entanglement formation between the single-particle states is shown. Both reflected and transmitted components of the scattered particle wavefunction are used to evaluate the quantum correlations between the incident carrier and the bound particle(s) in the dots. Our investigation provides a guideline for the analysis of decoherence effects due to the Coulomb scattering in semiconductor quantum dots structures.

Keywords: Quantum dots; entanglement; scattering.

1. Introduction

Recent advances in nanofabrication technology permit to design atom-like structures, such as quantum dots (QDs) and double quantum dot (DQDs), where electron states can be controlled and manipulated.12 Specifically, the charge states of QDs and DQDs have been shown to be excellent prototype blocks for the implementation of quantum-computing solid-state devices.54 Indeed, they are scalable to large system and compatible with current microelectronics technology.

A number of works address the entanglement production, control, and detection in single and double dots nanostructures on the basis of different physical mechanisms.56789 In all of them the most serious obstacle into generating entanglement and therefore performant quantum circuits is the interaction between the quantum system and its environment, resulting in the system decoherence. For charge qubits in QD and DQD the channels of decoherence are mainly two: the electron-phonon coupling and the electron-electron Coulomb interaction.10 The former, stemming from the interaction with the crystal lattice, is widely present in
all nanostructures even if its effects can be small at very low temperatures. The latter is due the coupling of the bound electrons in DQ and DQD to other carriers in the system and is therefore extrinsic.

In this work we analyze the entanglement formation due to two- and three-particle scattering events in QD and DQD structures, respectively. To this aim, we consider collisions between one or two electrons localized in a single or double dot and another electron entering the structure from a lead, and solve the corresponding Schrödinger equation of the two- or three-electron wavefunction in the real-space representation. In our numerical approach the scattering states are computed with the temperature of the system set equal to zero in order to realistically neglect the electron-phonon interaction. Specifically, we obtain the transmission (TC) and reflection coefficient (RC) of the electron crossing the nanostructure as a function of its initial kinetic energy and of the orbital state of the bound electron(s). We stress that the estimation of the amount of quantum correlations is a measure of the loss of coherence undergone by the charge qubits of the DQ and DQD when another carrier interacts with them.

2. The Physical Models

We compute the amount of quantum correlations between the scattered and the bound carriers interacting through Coulomb repulsion in two different systems, namely a single QD and a double QD, as described in the following.

2.1. Single-dot scattering

In this case we consider a quasi one dimensional structure where a potential profile $V_{QD}$ mimicking a QD is present. The system is sketched in the left panel of Fig. 1. The $N$ bound states and energies of the QD will be indicated as $|\Phi_n\rangle$ and $E_N$, respectively, while $|T_m^{(\langle\rangle)}\rangle$ describes the transmitted (reflected) electron with kinetic energy $T_m$. A single electron is localized in the QD ground state $|\Phi_0\rangle$ and interacts, via Coulomb potential, with a second electron incoming from the left lead with kinetic energy $T_0$. Specifically, we consider only cases in which $T_0$ is not sufficiently high to ionize the QD. Moreover the charging energy of the latter is assumed to be larger than the spacing between the the single-particle energy levels. This means that our system always operates in the two-particle regime.

The two-particle Hamiltonian $\mathcal{H}(x_1, x_2)$ is given by

$$\mathcal{H}(x_1, x_2) = -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x_1^2} - \frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x_2^2} + V_{QD}(x_1) + V_{QD}(x_2) + \frac{e^2}{4\pi\varepsilon r_{ij}},$$

where $r_{ij} = \sqrt{(x_i - x_j)^2 + d^2}$, $\varepsilon$ and $m^*$ indicate the dielectric constant and effective mass of the GaAs, respectively and $d$ is the cut-off term corresponding roughly to the lateral dimension of the confinement.

The two-particle scattering state $|\Psi\rangle$ is obtained by solving the time-independent Schrödinger equation $\mathcal{H}\Psi(x_1, x_2) = E\Psi(x_1, x_2)$ in the square domain.
Fig. 1. (Left panel) Potential profile $V_{\text{QD}}(x)$ of the QD structure: the potential well is 110 meV deep and 30 nm wide. (Right panel) Potential profile $V_{\text{DQD}}(x)$ of the double-dots structure: the two potential wells are each 110 meV deep and 30 nm wide and are separated by a 20 nm long barrier. In both cases the incident electron (I) arrives from the left lead while the bound electron(s) (B) initialized in the (D)QD ground state.

$x_1, x_2 \in [0, L]$ with $\mathcal{H}$ of Eq. 1. To this aim a generalization of the quantum transmitting boundary method is used. When the scattered particle leaves the simulation domain, i.e. after the scattering took place, the two-particle wavefunction reads

$$|\Psi_{\text{QD}}\rangle = \sum_{n=0}^{M} b_n |T_n^{<} \phi_n\rangle + \sum_{n=0}^{M} c_n |T_n^{>} \phi_n\rangle,$$

where the coefficients $b_n$ and $c_n$ represent the reflection and transmission amplitudes in the different energy levels, respectively, and the allowed energies $T_n$ of the scattered electron satisfy the energy conservation $E_0 + T_0 = E_n + T_n$. $M$ is the number of states for which $T_n$ is positive: for our choice of simulation parameters the contribution of the evanescent modes to the output state is found negligible. Here, all the travelling components of the scattered carrier, both reflected and transmitted, are taken into account in order to evaluate the appearance of quantum correlations and therefore no post-selection process is used, unlike other approaches.

The calculation of the entanglement between the single-particle states of the QD and the scattered particle can be performed by means of the von Neumann entropy $\xi_{\text{QD}}$ of the one-particle reduced density matrix $\rho_{\text{QD}}$ describing the bound electron. By tracing the two-particle density matrix $\rho = |\Psi\rangle \langle\Psi|$ over the degrees of freedom $|T_n^{<}\rangle$ of the scattered electron, we obtain $\rho_{\text{QD}}$ which takes a diagonal form. Its elements are given by $\rho_{\text{QD},nn} = |b_n|^2 + |c_n|^2$. Thus the von Neumann entropy can be expressed as:

$$\xi_{\text{QD}} = -\text{Tr}[\rho_{\text{QD}} \ln \rho_{\text{QD}}] = -\sum_{n=0}^{M} (|b_n|^2 + |c_n|^2) \ln (|b_n|^2 + |c_n|^2),$$
and is bound in the interval \([0, \ln(M + 1)]\), with \(\xi_{\text{QD}} = 0\) indicating no quantum correlations and \(\xi_{\text{QD}} = \ln(M + 1)\) indicating the maximum entanglement.

### 2.2. Double-dot scattering

In this subsection we describe the DQD system with three particles. Here, a Coulomb scattering between a carrier propagating in a quasi 1D GaAs channel with energy \(T_0\) and two electrons in a bound state of a potential structure \(V_{\text{DQD}}\) occurs. The potential \(V_{\text{DQD}}\) consists of two wells separated by a barrier and therefore mimicking a DQD device (see the right panel of Fig. 1). The two-particle bound states of the latter will be indicated as \(|\Gamma_n\rangle\) and their energies as \(\epsilon_N\). Unlike the single QD, some DQD energy levels can be degenerate. As initial condition, we take the two electrons in the ground state \(|\Gamma_0\rangle\).

The three-particle Hamiltonian \(H(x_1, x_2, x_3)\) reads

\[
H(x_1, x_2, x_3) = H_0(x_1) + H_0(x_2) + H_0(x_3) + \sum_{i=1}^{3} \sum_{j=1}^{i-1} \frac{e^2}{4\pi \varepsilon r_{ij}},
\]

where \(H_0(x_i)\) denotes the single-particle Hamiltonian

\[
H_0(x_i) = -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial x_i^2} + V_{\text{DQD}}(x_i).
\]

Also in this case, GaAs material parameters have been used in numerical calculations. By applying the few-particle version of the quantum transmitting boundary method to solve the Schrödinger equation with \(H(x_1, x_2, x_3)\), we find the reflection and the transmission amplitudes \(\beta_n\) and \(\alpha_n\), in analogy with the previous case, for the three-particle wavefunction:

\[
|\Psi_{\text{DQD}}\rangle = \sum_{n=0}^{M} \beta_n |T_{\Gamma_n}^-\rangle + \sum_{n=0}^{M} \alpha_n |T_{\Gamma_n}^+\rangle.
\]

Also in this case, the entanglement between the scattered carrier and the DQD system can be evaluated in terms of the von Neumann entropy \(\xi_{\text{DQD}}\) of the reduced density operator \(\rho_{\text{DQD}}\) describing the two bound electrons. Due to the degeneracy of some DQD energy levels, \(\rho_{\text{DQD}}\) is a diagonal-block matrix with the dimension of each block equal to the degree of degeneracy of the corresponding energy level and thus its diagonalization is required to calculate \(\xi_{\text{DQD}}\) in terms of the eigenvalues \(\lambda_n\) as \(\xi_{\text{DQD}} = -\sum_{n=0}^{M} \lambda_n \ln \lambda_n\).

### 3. Numerical Results

Here we present the numerical results and we analyze the relation between resonances in transmission and reflection spectra and the quantum correlations.

In the upper panel of Fig. 2 we report the von Neumann entropy \(\xi_{\text{QD}}\) as a function of the initial energy of the incoming carrier for the single-dot case, while in the lower panel the modulus of the RCs and TCs.
At low energy no correlations between the single-particle energy levels are found. In this case only a single channel is present for transmission and reflection: the incident carrier is scattered elastically (either transmitted or reflected) with energy $T_0$ while the QD is left in its ground state $\phi_0$. When the kinetic energy of the incoming carrier reaches a threshold value, around 12.5 meV, a new channel comes into play. Now, as a consequence of the scattering, the dot can also be excited in the first level $\phi_1$ with the energy of scatterer decreased to $T_1$. Starting from this energy, quantum correlations are built up between the particles and their peculiar behavior can be related to the resonances appearing in transmission and reflection spectra.\cite{8,9}

In order to get a better insight into such phenomena, a zoom of the above curves around a resonant energy $T_0=30$ meV is displayed in Fig. 3. The entanglement exhibits a maximum (where $\xi_{DQ}$ is around 0.6), when both the RC and TC of the second channel exhibit a peak. This means that the excitation probability of the DQ due to the collision becomes comparable to the probability of an elastic scattering, and this results in a significative increase in the lack of knowledge about the state of the electron bound in the dot.

Also the quantum correlations appearing in the DQD structure, as a consequence of the three-particle scattering event, can be related to the resonances in reflection and transmission spectra, as can be seen from Fig. 4. The maximum value of $\xi_{DQD}$ is reached when the initial energy $T_0$ of the incoming carrier is around 15.8 meV (see the detail expanded in Fig. 5). This peak occurs when the sum of the moduli of TC
Fig. 3. (Top) $\xi_{DQ}$ and (bottom) modulus of the TCs and RCs of the channels $T_0E_0$, $T_1E_1$ versus $T_0$, close to a resonant condition for the two-particle scattering of Fig. 2.

and RC describing the elastic scattering, i.e. when the DQD is left in its ground state $\Gamma_0$ with the scattered carrier in the energy level $T_0$, attains its minimum value while the probability that the scattering occurs through other channels is maximal. Therefore the energy levels of the DQD particles are correlated to the output energies of the scattered electron this meaning that a single pure state cannot be ascribed to the DQD system after the scattering.

4. Conclusions

In this paper we have calculated by means of the von Neumann entropy the amount of quantum correlations due to two- and three-electron scatterings in QD and DQD nanostructures, respectively. The outcomes of the numerical simulations show that the quantum entanglement between the scattered carrier and the particle(s) bound in the single or double dot systems is strictly related to the behavior of the TC and RC of the various scattering channels. Specifically, when the scattering occurs through various channels with comparable probabilities, the uncertainty about the specific energy states of the electrons bound in QD and DQD is increased due to the greater amount of entanglement with the scattered particle.

Our results agree with previous works where the entanglement formation due to the scattering events in single QDs is shown to be related to the different nature of the resonances present only in the transmission spectra of the injected carrier. There the entanglement is an estimation of the correlations showed up once
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Fig. 4. (Top) Von Neumann entropy $\xi_{DQD}$ and (bottom) modulus of the TCs and RCs of the channels $T_0 \psi_0$, $T_1 \psi_1$, and $T_2 \psi_2$, as a function of the initial energy of the incoming electron $T_0$ ranging from 10 to 40 meV, for the three-particle scattering in the DQD nanostructure.

Fig. 5. (Top) $\xi_{DQD}$ and (bottom) modulus of the TCs and RCs of the channels $T_0 \psi_0$, $T_1 \psi_1$ versus $T_0$, close to a resonant condition for the three-particle scattering of Fig. 4.
the crossing through the QD is successfully detected. On the other hand, in this work all the travelling components, either reflected or transmitted, of the scattered electron have been taken into account, that is no post-selection process has been considered. Thus our investigation can be viewed as the first step towards a rigorous analysis of the decoherence due to successive scatterings of a number of injected carriers, and therefore of an electric current.

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