Numerical study of 2-D quantum dots

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Abstract

We present a numerical study of the chemical potential and of the capacitance in a model quantum dot. Our model includes the electron-electron interaction and exchange and correlation effects within the framework of density functional theory. Our results exhibit the typical features observed in experiments, such as the increase in the capacitance for increasing number of electrons and the presence of irregularities in the succession of the chemical potential values vs. the electron number.

I. Introduction

Recent experimental results have shown extremely interesting single-electron phenomena in semiconductor quantum dots. The conductance across a quantum dot loosely coupled to the external electrodes via low-transparency tunnel barriers has been shown to be periodic with respect to the voltage applied to suitably positioned gates [1-3]. This effect has been explained as the consequence of the chemical potential in the dot lining up with the one in the external electrodes [2]. If the electrostatic energy prevails over the quantum confinement energy, the behavior of the dot is substantially capacitive and we expect evenly spaced values of the chemical potential versus the number of electrons. Several theoretical studies of quantum dots exist in the literature [4-5], dealing with both very idealized models and with realistic, three-dimensional models. Our aim has been to solve for the chemical potential in a structure which, even though simplified, retains all the characteristic features observed in the experiments. We study a 2-D model quantum dot defined by a given confining potential. Except for this simplification, i.e. the confining potential not determined from the actual characteristics of the semiconductor layers and the geometries and voltages of the metal gates, we try to take into account all relevant contributions, including many-body effects, within the framework of density functional theory.

II. Quantum dot model

Our model quantum dot is two-dimensional and defined by the shape of the confining potential, represented by hard walls along the perimeter of a square region to which we shall refer in the following as "quantum box". The potential within the box is not constant, but quasi-parabolic, as the one produced by a positive background charge of $100q$ (q being the electron charge), uniformly distributed over the surface of the box.

The potential effectively seen by the electrons in the calculations presented in this paper is substantially the quasi-parabolic part, since this already provides enough confinement as to make the electron density vanish before reaching the hard walls. This is a realistic approximation of the actual potential in the experimental situations.
Our study is performed at the temperature of 0 K, thus for a system in the ground state. We solve for the eigenfunctions and the eigenenergies of the quantum dot by means of an iterative, self-consistent procedure [8] based on the Kohn-Sham density functional approach [9].
The Schrödinger equation is discretized with a standard five-point formula and the eigenvalues and eigenvectors of the matrix thus obtained are computed by means of a Ritz iterative procedure.

III. Numerical results

The chemical potential is the main quantity we want to evaluate. Once the wave functions and the energy eigenvalues have been determined, there are several ways to obtain the chemical potential $\mu(N)$ (N being the number of electrons). We can compute the total energy $E(N)$ of the system from [9]

$$E(N) = \sum_{i=1}^{N} \varepsilon_i - \frac{1}{2} \int \int \frac{n(\vec{r}) n(\vec{\rho})}{|\vec{r} - \vec{\rho}|} d\vec{r} d\vec{\rho} + \int n(\vec{r}) \left[E_{ex}(n(\vec{r})) + E_{corr}(n(\vec{r})) - V_{ex}(n(\vec{r})) - V_{corr}(n(\vec{r})) \right] d\vec{r}, \qquad (1)$$

where ε_i are the energy eigenvalues for each electron, $n(r)$ is the total electron density, $E_{ex}, E_{corr}, V_{ex}, V_{corr}$ are the exchange and correlation energies and potentials, respectively.
From the definition of chemical potential we have that $\mu(N) = E(N) - E(N-1)$. The result of this differentiation, however, may be adversely affected by numerical errors in the values of $E(N)$ and $E(N-1)$. A plot of μ versus N obtained with this procedure for a 60×40 nm box is shown in Fig. 1 with solid dots. In the same figure we report, with empty squares, the chemical potential computed for the same structure with a different method: Slater's approximation. The "removal energy", i.e. the energy needed to remove one electron from a system of interacting electrons can be approximated [10] by $\varepsilon(N + 0.5)$, the energy eigenvalue for a fictitious additional particle with charge $q/2$. It is apparent that for a small number of electrons both methods yield the same result while, for more than 10 electrons, the technique based on the difference between the total energies for N and $N - 1$ electrons starts being severely affected by numerical noise. We have therefore used Slater's approximation in most of our calculations.
In Fig. 2 we report an idealized representation of the conductance peaks which would be measured between two leads very loosely coupled through the a square quantum box of various sizes. The height of the peaks is purely conventional and there is no broadening because of the assumption of 0 K temperature and of vanishingly small transparency for the tunnel barriers. The three plots correspond to three different box sizes: 40×40 nm, 80×80 nm and 200×200 nm.

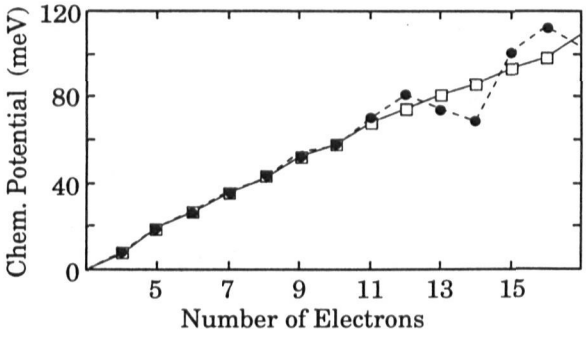

Fig. 1 Chemical potential vs. number of electrons

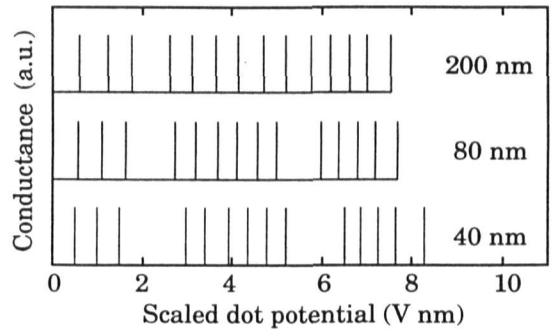

Fig. 2 Conductance peaks for a square quantum box

The quantity on the abscissae axis is the dot potential scaled multiplying it by the length of the box side in nanometers. This scaling normalizes the three plots with respect to the energy associated with the Coulomb interaction [1]. The first peak, coincident with the zero reference for the dot potential, is for three electrons.

The spacing between conductance peaks is very uneven for the smallest box and a more careful exam of the plot shows that there are groups of evenly spaced peaks corresponding to the various degenerate energy levels in the square box. For example, the peaks for the 3rd, 4th, 5th and 6th electrons correspond to to the 2nd and 3rd single-electron orbitals, which are degenerate in a square box, in the absence of electron-electron interaction.

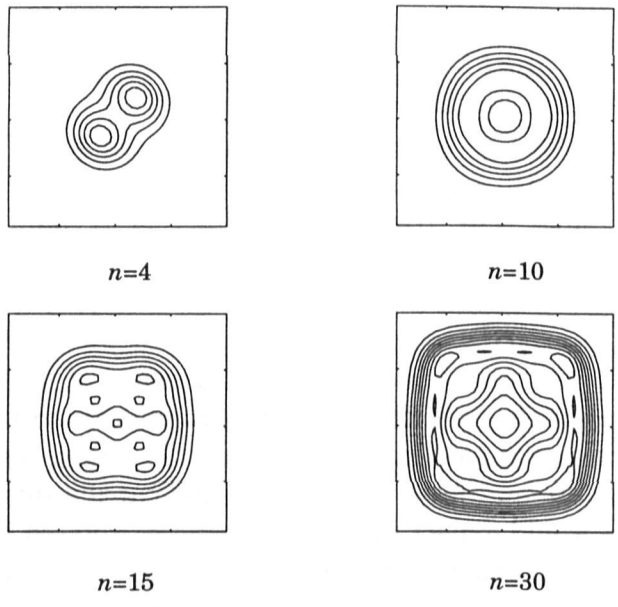

Fig. 3 Electron density in a square quantum box.

As the size of the dot increases, we observe a reduction of the relative importance of the quantization energy and the clear prevalence of the Coulomb energy, leading to an almost even spacing for the 200×200 nm box. The plot for this largest box also shows an effect which has been experimentally observed: the reduction of the average spacing between peaks with increasing number of electrons. This effect is mainly due to the increase of the area of significant electron density when more electrons are added to the

dot and see a less attractive potential, because of the screening performed by the ones in the lower orbitals.
In Fig. 3 contour plots of the electron density are shown for a number of 4, 10, 15, 30 electrons confined in a 120 × 120 nm quantum box. There is a very significant change in the extension of the non-zero electron density and in its shape when the number of electrons is increased. This accounts for the observed crowding of conductance peaks.
A differential capacitance C_d can be associated with a quantum dot, according to the following definition:

$$C_d(N) = \frac{q^2}{\mu(N+1) - \mu(N)}. \tag{2}$$

This quantity is more readily understandable if we consider a dot in the proximity of some conducting surface such as, for example, a metal gate. This is also the most common configuration in the devices which have been experimentally investigated. The differential capacitance represents the ratio of the electron charge to the variation of the voltage between the gate and the dot when an electron is added to the system. If the gate is much larger than the dot, it can be approximated with an infinite conducting surface and modelled with properly placed image charges.

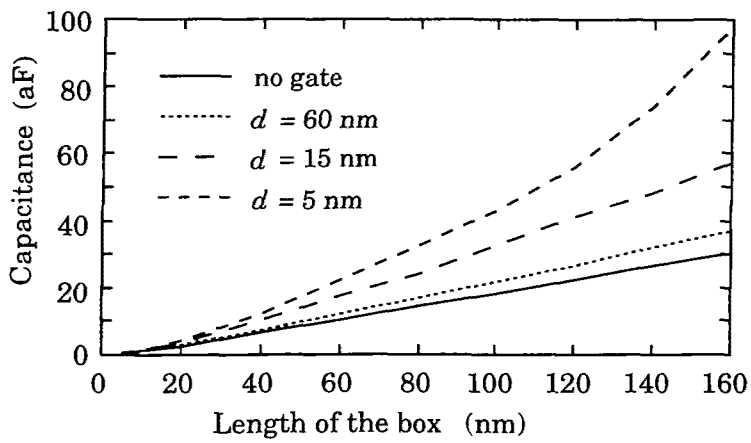

Fig. 4 Capacitance vs. length for 4 electrons.

The results of our calculations of the capacitance [8] in the presence of metal gates are shown in Fig. 4. The four curves are for 4 electrons in a rectangular quantum box with a length/width ratio of 4/3 and a metal gate at a distance d of 5, 15, 60 nm or no gate at all. We see that, while for no gate and for a distant gate the capacitance grows in a substantially linear fashion as we would expect for a 2-D geometry isolated in 3-D space (see e.g. [2]), for a very close gate the behavior becomes almost quadratic, reaching the well-known classical limit of the parallel plate capacitor. For a small gate-dot separation we perform simply a Hartree calculation, because the expressions used for the exchange and correlation potentials [8] do not hold in the presence of strong interaction with the image charges.

IV. Conclusion

We have studied a model two-dimensional quantum dot with a quasi-parabolic confining potential, including many-body effects within a density functional approach. Results for

the chemical potential in a square box have been presented, showing the transition from a behavior dominated by quantum effects to one in which the Coulomb charging energy is predominant. The differential capacitance which can be thus defined approximates the one of a conducting 2-D surface with a shape like the one of the area of significant electron density in the quantum dot.

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