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Theoretical study of electron confinement in three-dimensional quantum dots using variational Monte Carlo methods

C. Ramírez[3], R. Díez Muiño[1,2] and W. Schattke[2,3]

[1] Unidad de Física de Materiales, Centro Mixto CSIC-UPV/EHU,
P. Manuel de Lardizabal 3, 20018 San Sebastián, Spain
[2] Donostia International Physics Center DIPC,
P. Manuel de Lardizabal 4, 20018 San Sebastián, Spain
[3] Institut für Theoretische Physik, Christian-Albrechts-Universität
Kiel, Leibnizstraße 15, D-24118 Kiel, Germany

Abstract. We use the variational quantum Monte Carlo method to calculate the electronic properties of a three-dimensional quantum dot of cubic size. We put special emphasis in the calculation of the electron pair-correlation function $g(\mathbf{r}_1, \mathbf{r}_2)$ as a typical two-body quantity in which correlation effects are of much importance. We show results for different quantum dot sizes, keeping the electronic density unvaried. The relevance of this work in connection to geminal-based approximations of electron-electron effective potentials in electronic media is also discussed.

Introduction

In the last twenty years, experimental advance in semiconductor processing techniques has fueled the development of a new subfield in condensed matter physics, namely the study of nanometer-sized systems with only a few active electrons [1, 2]. These systems are usually called quantum dots (QD), as a reference to the quantum confinement of the electrons in the three dimensions of space. The relatively small number of electrons contained in a single QD, as well as the discretization of its one-electron levels, make it behave as an artificial atom in many respects. This similarity is present, for instance, in the QD many-body properties, drastically modified when a single electron is added to (or removed from) the system. One of the most appealing features of QDs is that many of these electronic properties can be designed and artificially controlled in the laboratory, making them specially fit for the search of nanosized materials with properties at wish. Potential technological applications of QDs in semiconductor industry, spintronics, and quantum computing, among others, are thus vast.

From the fundamental point of view, QDs are very attractive systems to study electron correlation properties, as they are midway between bulk condensed matter and gas-phase atoms. Hence much of the theory of electron correlation in atomic physics has been succesfully applied to these condensed-matter systems. They have also become a sort of test to many of the standard many-body theories (density functional theory, Hartree-Fock, quantum Monte Carlo, etc.) currently used for the description of matter. Shell structure, spin polarization and Coulomb blockade are clear examples of QD properties under active scrutiny in the last years.

In this short paper, we focus in one of the basic magnitudes describing the electronic properties of many-body systems, namely the electron pair-correlation function, which is a typical two-body quantity. The pair-correlation function $g(\mathbf{r}_1, \mathbf{r}_2)$ can be defined as the probability of finding one electron at the position $\mathbf{r}_2$ when there is already another electron at $\mathbf{r}_1$. We study the shape of $g(\mathbf{r}_1, \mathbf{r}_2)$ in a three-dimensional (3D) QD, and analyze its dependence on the system size. The behavior of $g(\mathbf{r}_1, \mathbf{r}_2)$ gives us some insight on the influence of electron confinement in the electron-electron interaction properties.

1. Monte Carlo computational method

Quantum Monte Carlo methods have been widely used for the study of the electronic structure of QDs [3]. Our model system is a 3DQD of cubic shape with lateral dimension of length L. A fixed number of electrons N is confined to the dot, making the average electronic density equal to $n_0 = N/L^3$ (effective atomic units are used throughout this manuscript: $\hbar = e^2/\epsilon = m^* = 1$, being m^* the electron effective mass and ϵ the dielectric constant of the medium). As customary, we also define the average one-electron radius r_s from $1/n_0 = 4\pi r_s^3/3$. We approximate the confining potential of the 3DQD $V(\mathbf{r})$ as a constant potential $V(\mathbf{r}) = 0$ inside the dot and an infinite potential $V(\mathbf{r}) = \infty$ elsewhere.

We use the variational Monte Carlo method (VMC) to calculate the many-body electronic wavefunction Ψ [4, 5]. For this purpose, we build a parametrized wavefunction in the following way:

$$\Psi = D^{\uparrow} D^{\downarrow} \exp\left[-\sum_{i<j} u(\mathbf{r}_{ij})\right], \tag{1}$$

where i is an index running over all electrons in the system, the $D^{\uparrow}$ and $D^{\downarrow}$ factors correspond to determinants for spin up and spin down electrons respectively, and the function $u(\mathbf{r})$ is a two-body Jastrow factor:

$$u(\mathbf{r}) = \frac{\alpha}{\beta + r}, \tag{2}$$

where β is fixed by the cusp condition and α is a variational parameter that is used to minimize the total energy of the system.

The determinants $D^{\uparrow}$ and $D^{\downarrow}$ in Eq. 1 are made from single-particle wavefunctions $\phi(\mathbf{r})$, that we approximate by:

$$\phi(\mathbf{r}) = A\, sin\left(\frac{n_x \pi x}{L}\right)\, sin\left(\frac{n_y \pi y}{L}\right)\, sin\left(\frac{n_z \pi z}{L}\right), \tag{3}$$

where each of the $\mathbf{r}$ coordinates (x, y, z) is confined between 0 and L, and A is a normalization factor. In the following, we neglect the dependence of the wavefunction on the

z-component, as a preliminary test for further studies on the electronic properties of quasi two-dimensional quantum dots.

After optimization of this wavefunction following a variational procedure, the expectation value of any observable $\hat{O}$ can be calculated from:

$$< \Psi|\hat{O}|\Psi > \;=\; \frac{1}{M}\sum_{i=1}^{M}\frac{\hat{O}\Psi(\mathbf{R}_i)}{\Psi(\mathbf{R}_i)}, \quad (4)$$

where the set $\mathbf{R}_i$ represents a N-particle coordinate configuration, that we sample by means of the Metropolis algorithm.

In the following, we use this numerical method to calculate the electron pair-correlation function in the 3DQD. For the sake of simplicity, we use the center of mass spatial coordinates, $\mathbf{r} = (\mathbf{r}_1 - \mathbf{r}_2)$ and $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$, so that the pair-correlation function becomes $g(\mathbf{r}, \mathbf{R})$. Furthermore, we perform an average over the QD volume (i.e., over the $\mathbf{R}$ coordinate), from which we define by a spherical average the function $g(r)$.

2. Pair correlation function

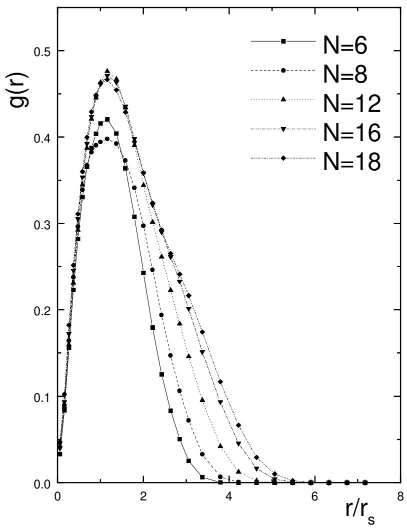

Fig. 1. Pair-correlation function $g(r)$ as function of spatial coordinate r, for five QDs of different sizes. Spatial coordinate r is normalized to r_s. Number of electrons N for each dot is shown in inset. Average electronic density is kept constant (see text for further details).

Let us show in Fig. 1 the pair-correlation function $g(r)$ for several QDs, with a different number of electrons N confined in each of them. We have kept a constant average value of the electronic density in all calculations ($r_s = 3.25$), by varying the QD volume L^3. The pair-correlation function $g(r)$ is very small for small electron distances, as a consequence of both the Pauli principle and Coulomb repulsion. It includes only contributions from antiparallel spin electrons. The behavior of $g(r)$ close to the origin is very similar for all QD sizes and no dependence on the boundary conditions is found. At large distances, for which the value of the pair-correlation function saturates in the homogeneous electron gas, $g(r)$ obviously vanishes due to the finite size of the QD. The general shape of $g(r)$ is shrinked in the case of smaller QDs, but the maximum of $g(r)$ appears in all cases at the same distance from the origin $r \approx 1.1r_s$. Hence we can conclude that the short-order spatial distribution of the electrons is not significantly affected because of the change in the confinement dimensions and does not depend on the size of the system, provided that the electronic density of the system is kept constant.

3. Discussion and Outlook

Our results for the pair-correlation function $g(r)$ in a 3DQD are averaged over spin components. Nevertheless, more complete information about electron correlation can be achieved by calculating separately the spin-dependent pair-correlation functions for parallel [$g_{\uparrow\uparrow}(r)$ and $g_{\downarrow\downarrow}(r)$] and antiparallel spin [$g_{\uparrow\downarrow}(r)$ and $g_{\downarrow\uparrow}(r)$]. Recently, much theoretical effort has been dedicated to the study of electron-electron effective interactions in homogeneous systems via the geminal representation [6, 7, 8]. The calculation of the spin-dependent pair-correlation functions in 3DQD would allow to add some information on the influence of electron confinement in the effective spin-dependent interaction potential between electrons.

Furthermore, the understanding of the electronic properties of QDs in their ground state have very much advanced in the last years. However, many unknowns still remain in the description of excited states, electron dynamics, and electronic response properties. Quantum Monte Carlo methods, either alone (diffusion Monte Carlo, for instance) or in combination with other approximations, are one of the most promising methods to address this kind of problems. Work along these lines is currently in progress.

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