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Two interacting electrons in low-lying states in a spherical quantum dot

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ABSTRACT

The energy spectra of two electrons in low-lying excited states in a spherical quantum dot are estimated with different barrier heights. The screened electron–electron interaction is treated through a dielectric function and the correlation energy is calculated for different dot sizes. The two electron problem is also treated as an effective one body problem. It is found that: (i) correlation effects are significant for smaller dots, (ii) spatial-dependent screening function does not lead to appreciable changes in binding energies, (iii) the effects of barrier height is appreciable on confinement and it has no effect on correlation energy of electrons and (iv) the effect of binding energy for smaller dots is substantial when included the correlation effect more than treated as one body problem.

1. Introduction

The study of semiconductor quantum dots (QDs) and nanocrystals have been of a great interest from the experimental and theoretical point of view in recent years [1]. The origin of the interest lies in the size of quantization in solids and in those objects. The electron spectrum of an ideal QD comprises a set of discrete levels. This makes the semiconductor QD very important in the applications of optical and transport properties of semiconductors. In these quasi-zero-dimensional systems in which the carrier motion is restricted to a narrow region of a few nanometers in dimension, the correlation among the electrons are shown to be appreciable [2]. Few electron QD have been the subject of intensive research activities recently [3–5]. The interplay of electron–electron interaction plays a vital role in two electrons in a QD and hence it is especially interesting. Other physics of two electrons in semiconductor QD has been intensively investigated in the past few years. Most of the calculations use infinite barrier models with either square well potential confinement [6] or parabolic confinement [7].

Works on finite barrier confinement with square well potential are sparse [8]. However, the binding energies of two electrons in a spherical QD with square well potential confinement have been considered recently [9]. Bryant [10] studied the energy levels for two electrons in a square quantum well box. While the effect of dielectric mismatch between the dot material and the surrounding has been considered by Brus [11] and Cantele et al., [12] for the CdS and CdSe dots, respectively, the effect of anisotropy in the ellipsoidal-shaped QD has been thoroughly investigated in Ref. [13]. Zhu et al., [14] have pointed out the significance of size and shape effects on electron–electron interactions in a parabolic confinement. Bester and Zunger [15] predict interesting results in the study of spectra of charged QD. Studies on singlet–triplet splitting, degree of entanglement and correlation in InAs/GaAs QD molecules are discussed in Ref. [16]. Significance of dielectric mismatch on electron and hole addition spectra in InAs, InP and Si dots has been investigated using a pseudo-potential formalism by Franceschetti and Zunger [17].

Blanter et al., [18] calculated energy spectra of two-dimensional two electron QD in transverse magnetic field by numerical diagonalizing of the Hamiltonian on the basis of single-particle eigenfunctions. Two electron system of two adjacent QD with a two-dimensional parabolic lateral confining potential, and of two coupled or double, spatially separated QDs (a "horizontal" and a "vertical" QD molecule), and of their behavior in an external transverse magnetic field is studied by Kaputkin and Lozovik [19]. Coupled QD are studied by Rontani et al., [20] who showed that the transitions between different quantum phases could be induced through the inter-dot coupling both for a system of few electrons (or holes) and for aggregates of electrons and holes. The spin configurations of a spherical QD, defined by a three-dimensional (3D) harmonic confinement potential, containing a few Coulomb Fermi particles (electrons or holes) are studied by Sundqvist et al., [21]. El-Said [22] has recently studied the relative

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Hamiltonian of two interacting electrons confined in a QD by the shifted 1/N expansion method. Xie [23] has studied three electrons confined in one-, two- and three-layer QD, by the exact diagonalization method who investigated the ground-state electronic structures and angular momentum transitions. The electronic structures of N QD molecules are investigated theoretically in the framework of effective-mass envelope function theory by Li and Xia [24] recently.

Transport and optical spectroscopy have revealed field-tunable rich phases in few electron QD systems. Hence, it is important to calculate the low-lying states in the presence of confinement and electron–electron correlation. The electron–electron interaction effects include the mutual Coulomb term and spin part. In the present work, we have considered a GaAs QD embedded in a $Ga_{1-x}Al_xAs$ matrix with finite barriers. When two electrons are introduced into the dot, we variationally estimate the total energy of the system , assuming spherical well potential for confinement for different barrier heights. The screened electron–electron interaction is treated through the dielectric screening function obtained by Richardson and Vinsome [25]. The two electron problem is also treated as an effective one body problem with the Hamiltonian. The models and calculations are provided in Section 2, while the results and discussion are given in Section 3.

2. Theory

2.1. Single electron in a spherical QD

We consider two interacting electrons of effective mass m^*, which is $0.067m_0$ for GaAs, the system is described by the Hamiltonian

$$H=\sum_{j=1}^{2}\frac{\bar{p}_j^2}{2m^*}+V_D(\bar{r}_j) \tag{1}$$

where $V_D(\bar{r})$ is the barrier height given by $V_D(\bar{r})=Q_c\Delta E_g(x)$. Q_c is the conduction band offset parameter, which is taken to be 0.658 and the band gap difference between GaAs and $Ga_{1-x}Al_xAs$ is given by

$$\Delta E_g(x)=1.155x+0.37x^2\ \text{eV} \tag{2}$$

The units of length and energy used throughout the present paper are the effective Bohr radius $R^*=\hbar^2\varepsilon_0/m^*e^2$ and $R_y^*=m^*e^4/2\varepsilon_0^2\hbar^2$, where ε_0 is the static dielectric constant of GaAs.

The eigenfunctions for the three lowest lying states within the dot are given by

$$\psi_{1s}(\bar{r})=\begin{cases}N_1\dfrac{\sin(\alpha_1 r)}{r}, & r<R\\ N_2\dfrac{e^{-\beta_1 r}}{r}, & r\geqslant R\end{cases} \tag{3}$$

$$\psi_{1p}(\bar{r})=\begin{cases}N_3\left[\dfrac{\sin(\alpha_2 r)}{(\alpha_2 r)^2}-\dfrac{\cos(\alpha_2 r)}{\alpha_2 r}\right]\cos\theta, & r<R\\ N_4\left[\dfrac{1}{\beta_2 r}+\dfrac{1}{(\beta_2 r)^2}\right]e^{-\beta_{21}r}\cos\theta, & r\geqslant R\end{cases} \tag{4}$$

$$\psi_{1d}(\bar{r})=\begin{cases}N_5\left[\left(\dfrac{3}{(\alpha_3 r^2)^3}-\dfrac{1}{\alpha_3 r}\right)\sin(\alpha_3 r)-\dfrac{3}{(\alpha_3 r)^2}\cos(\alpha_3 r)\right] & r<R,\\ (3\cos^2\theta-1)\\ N_6\left[\dfrac{1}{\beta_3 r}+\dfrac{1}{(\beta_3 r)^2}+\dfrac{1}{(\beta_3 r)^3}\right]e^{-\beta_{31}r}(3\cos^2\theta-1) & r\geqslant R\end{cases} \tag{5}$$

where $N1$, $N2$, $N3$, $N4$, $N5$ and $N6$ are normalization constants and $\alpha 1$ and $\beta 1$ are given by

$$\alpha_1=\sqrt{2m^*E_1}\ \text{ and }\ \beta_1=\sqrt{2m^*(V_D-E_1)} \tag{6}$$

Matching the wavefunctions and their derivatives at the boundary $r=R$, the energy eigen values are determined by imposing the boundary conditions

$$-\frac{i\hbar}{m^*}\frac{\partial\psi}{\partial r}(r<R)|_{r=R}=-\frac{i\hbar}{m^*}\frac{\partial\psi}{\partial r}(r\geqslant R)|_{r=R} \tag{7}$$

Using Eqs. (4)–(7), we obtain

$$\alpha_1 R+\beta_1 R\tan(\alpha_1 R)=0\ \text{ for } s\text{-states} \tag{8}$$

$$\frac{\cot(\alpha_2 R)}{\alpha_2 R}-\frac{1}{(\alpha_2 R)^2}=\frac{1}{\beta_2 R}+\frac{1}{(\beta_2 R)^2}\ \text{ for } p\text{-states} \tag{9}$$

and

$$\begin{aligned}&9\alpha_3 R-(\alpha_3 R)^3+[4(\alpha_3 R)^2-9]\tan(\alpha_3 R)\\ &\quad=-[(3-(\alpha_3 R)^2\tan(\alpha_3 R)-3(\alpha_3 R)]\\ &\qquad\times\left[\frac{(\beta_3 R)^3+4(\beta_3 R)^2-9}{(\alpha_3 R)^2+3\alpha_3 R+3}\right]\ \text{ for } d\text{-states}\end{aligned} \tag{10}$$

Solving these transcendental equations, the confined particle energies $E_l^{(n)}(n=1,2,3,\ldots,l=0,1)$ are obtained. Similar equations may be obtained for other excited states, $l=2,3\ldots$ The confinement energies of the first three states are drawn in Fig. (1).

2.2. Two electrons in a spherical QD

The Hamiltonian for this system is

$$H=\sum_{j=1}^{2}\left\{\frac{\bar{p}_j^2}{2m^*}+V_D(\bar{r}_j)\right\}+\frac{e^2}{\varepsilon_0|\bar{r}_1-\bar{r}_2|} \tag{11}$$

where $V_D(\bar{r})$ is expressed as above. The second term is the Coulomb interaction energy which is calculated numerically here.

Considering s-states and p-states, the triplet state energies are obtained using the wavefunctions $\psi_{1s-1s}(\bar{r}_1,\bar{r}_2)$, $\psi_{1s-1p}(\bar{r}_1,\bar{r}_2)$ and $\psi_{1s-2s}(\bar{r}_1,\bar{r}_2)$, as expressed above. The electron–electron interaction is included through a dielectric function which was worked out by Richardson and Vinsome [25]. This function is given by

$$\varepsilon(\bar{r})=(a_1+a_2e^{-b_1 r}+a_3e^{-b_2 r})^{-1} \tag{12}$$

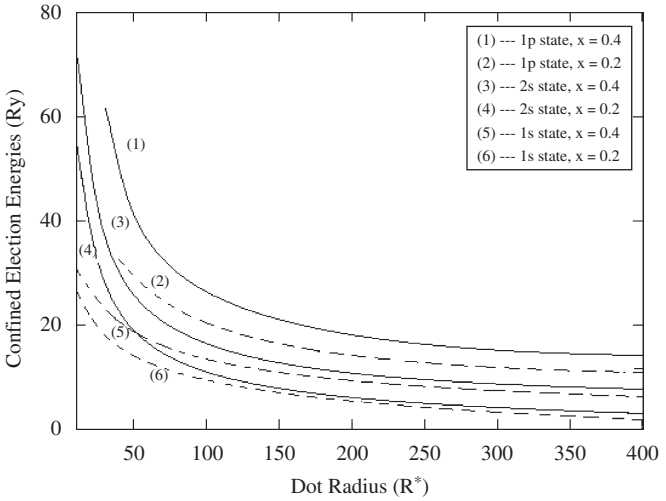

Fig. 1. Variation of confined energies with the dot radius for two different concentrations in the infinite barrier model.