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Exchange and Coulomb interactions of two electrons in double ellipsoidal quantum dots

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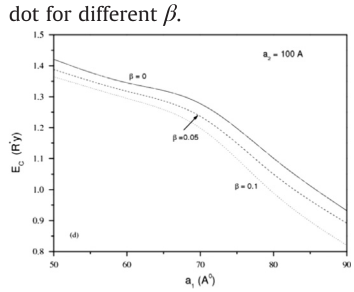
HIGHLIGHTS

- A suitable change of variable transforms the ellipsoidal quantum dot into the spherical QD.
- The energy levels and wave function of two-electron system are calculated.
- The exchange energy versus semi-axis of ellipsoidal quantum dot is calculated.
- The time evolution of two-electron wave function is studied.
- The Coulomb energy in terms of ellipticity constant is calculated.

GRAPHICAL ABSTRACT

The variations of Coulomb energy of two electrons system versus semi-axis of the ellipsoidal quantum dot for different β.



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ABSTRACT

The present study seeks to scrutinize the interactions of two electrons on the electronic properties of double ellipsoidal quantum dots (EQD). In this regard, the effective-mass approximation within a perturbation scheme is used and the Coulomb and exchange energies of the two electrons ellipsoidal quantum dot are calculated for GaAs/GaAlAs/AlAs structure. The results showed that the Coulomb and exchange energies depend not only on the thickness of the intermediate layer but also on the ellipticity constant.

1. Introduction

The study of semiconductor quantum dots (QD) and nanocrystals has been of 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 quantum dot comprises a set of discrete levels. This makes the semiconductor quantum dot very important in the applications of optical and transport properties of semiconductors. The physical properties of the controlling quantum dot are attractive not only from the fundamental scientific point of view, but also because of its potential application in the development of semiconductor optoelectronic devices [2].

In theoretical works, it is customary to assume a spherical shape for the quantum dot. Since deformation of spherical shape during quantum dot growth is unavoidable, quantum dot with other shapes is achieved through probability. The ellipsoidal shape may be a better representation of the actual problems [3,4].

The electronics properties of quantum structures confined in other nano-structures have attracted many researchers for their experimental applications. Theoretical study of multilayered nanostructures originates from works done by Pietiläinen and Chakraborty [5]. In this work, they studied few electron states in two-dimensional nanorings. Study of impurity binding energy of a multilayered spherical GaAs/(Ga, Al)As quantum dot by Aktas and

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Boz [6], three dielectric layer model for the interface between a spherical quantum dot and the surrounding matrix by Deng [7], the binding energy of an impurity located at the center of multi-layered quantum dot (MSQD) by Boz et al. [8] are a few examples of some interesting investigations in this field.

The energy levels of few electrons quantum dots with finite confinement potential were obtained by Fong et al. using the local density approximation [9]. In the infinite confinement potential, the excess electrons in quantum dots are always bound and possess only discrete energy levels. But in the real quantum dots structures, the confining potential is finite and the number of electrons which can be accumulated in a given quantum state of a quantum dot, the capacity of dot, can be determined [10]. It has been shown that electron correlation plays a significant role in quantum dots. There have been considerable efforts on the estimation of correlations in few electron quantum dots. Zhu et al. [11] have pointed out the significance of size and shape effects on electron–electron interactions in a parabolic confinement. The energy spectra of two electrons in low-lying excited states in a spherical QD with different barrier heights are studied by John Peter and Saravana Kumar [12]. Correlation energies in a triplet state of a two electrons spherical QD with square well potential confinement are estimated in Ref. [13]. Two electronic states and state exchange time control in multilayered spherical quantum dot with infinite confinement potential are investigated in [14]. Effect of tilted magnetic field on energy levels of two-electron quantum dots with harmonic and hard-wall potential is presented in [15].

The aim of this work is to study the electron–electron interactions in multilayered ellipsoidal quantum dots with finite confining potential. The Coulomb and exchange interaction energies of two electrons located at the GaAs ellipsoid with GaAlAs coating in the environment *AlAs* surrounding the system are calculated (Fig. 1). The outline of the paper is as follows: in Section 2 the Schrödinger equation solved for a two electron system in an ellipsoidal quantum dot confined in other EQD, held at a finite potential. The ground state energy and wave function are calculated by applying the boundary conditions at the interfaces, then using the perturbation method, the Coulomb and exchange energies are calculated. Section 3 contains our results and discussions. Finally, the conclusions are presented in Section 4.

2. Theory

In the effective mass approximation, the Hamiltonian of two electrons in double ellipsoidal quantum dots (EQD) can be written as

$$H = H_1 + H_2 + H_{12} \tag{1}$$

where

$$H_{1,2} = \frac{\hat{P}_{1,2}^2}{2m^*} + V(R) \tag{2}$$

m^* and $V(R)$ are the position-dependent of the effective mass and the confinement potential, respectively. H_{12} is the Coulomb interaction potential of two electrons and is given by

$$H_{12} = \frac{e^2}{\varepsilon_d |\vec{R}_1 - \vec{R}_2|} \tag{3}$$

where ε_d is the dielectric constant of nanolayer. For an EQD with circular cross-section in the X, Y-plane the ellipticity constant is

$$\beta = 1 - \frac{a}{c} \tag{4}$$

where a and c are the semi-axes of the ellipsoid. It is useful to change the variables as follows [16]:

$$X \to \frac{ax}{r_0}, \quad Y \to \frac{ay}{r_0}, \quad Z \to \frac{cz}{r_0}, \ r_0 = (a^2c)^{1/3} \tag{5}$$

This change transforms the ellipsoid into a sphere of radius r_0, with the same volume. After these coordinate transformation the Hamiltonian is given as

$$H = h_1 + h_2 + h^* + \Delta h + \Delta V(r) \tag{6}$$

where

$$h_{1,2} = \frac{p_{1,2}^2}{2m^*} + V(r), \tag{7}$$

$$\Delta h = \sum_{j=1}^{2} \frac{\beta}{3m^*}(\hat{p}_j{}^2 - 3\hat{p}_{j,z}{}^2). \tag{8}$$

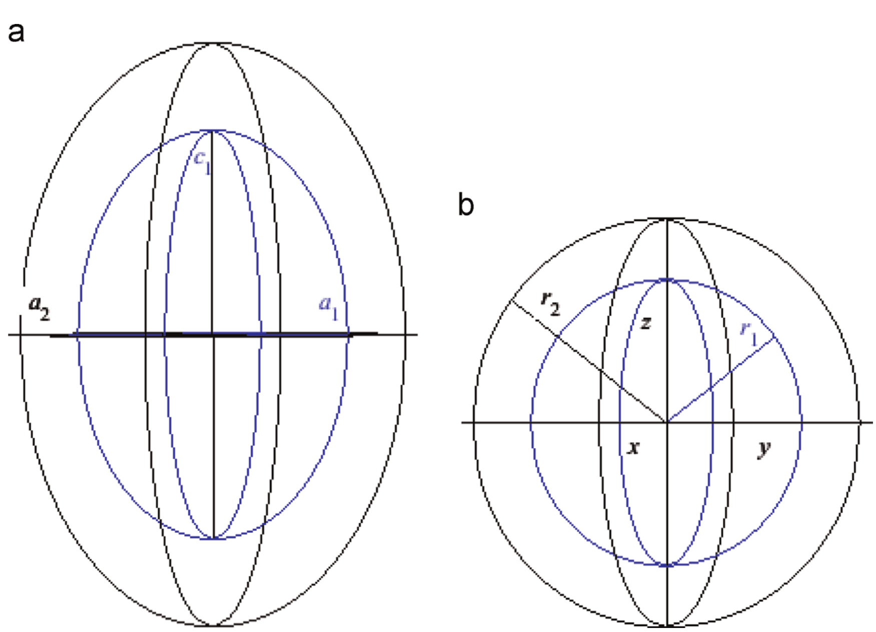

Fig. 1. A schematic representation of double ellipsoidal quantum dots. (a) Original structure and (b) the transformed coordinate.