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Effect of dielectric mismatch on impurity binding energy in double ellipsoidal quantum dots

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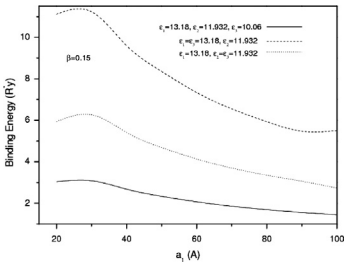
HIGHLIGHTS

- Binding energy of hydrogenic impurity in double ellipsoidal quantum dot (DEQD) is calculated.
- Effect of dielectric mismatch due to different regions on the binding energy in DEQD is investigated.
- Effect of self polarization energy due to the interaction of charge with its induced charge is considered.
- Surface polarization charges reduce the energy of carriers.
- Self polarization energy increases the electron energy.

GRAPHICAL ABSTRACT

The variation of binding energy versus semi-axis of the ellipsoidal quantum dot for different dielectric constants of well and barrier regions.



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ABSTRACT

The present study seeks to scrutinize the effect of polarization charges on the electronic properties of double ellipsoidal quantum dots. In this regard, the effective-mass approximation within a variational scheme is used and the binding energy of hydrogenic impurity located at the center of ellipsoidal quantum dot (EQD) is calculated for GaAs/GaAlAs/AlAs structure. The effect of surface polarization charges due to impurity and self-polarization charges on the binding energy is considered. The results showed that the binding energy depends not only on the thickness of the intermediate layer but also on the ellipticity constant.

1. Introduction

The study of low-dimensional systems has been an interesting subject of investigation in recent years [1]. Because of quantum size effects in these structures, the physical properties of confined quantum systems strictly depend on the external shape of the system under consideration. In theoretical works, it is customary to assume a spherical shape for the quantum dot (SQD). Since deformation of spherical shape during quantum dot growth is unavoidable, other shapes of quantum dot (QD) are probably achieved. The ellipsoidal shape may be a better representation of the actual problems [2,3].

Impurities have important effects on physical characteristic in low-dimensional semiconductor systems. The impurity changes the energy levels of the materials and therefore, the electronic and optical properties are affected [4]. A significant number of studies have been carried out on calculation methods of impurity states in nanostructures [5–10]. In many of the investigations devoted to the calculation of binding energy in nanostructures, the dielectric constant mismatch between different regions of a system was not considered. When the dielectric constant changes abruptly across the heterojunction, the discontinuity of the square quantum well model implies an infinite internal electric field at the heterojunctions,

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which is not physically possible. In reality, the parameters such as dielectric constant and effective mass change over a few monolayers for a perfect microscopic interface [11]. There are also a number of works done on the polarization charges in nanostructures. The effect of dielectric mismatch on binding energy in quantum well and quantum wire is investigated in Refs. [12–14]. Coulomb interaction in thin semiconductor and semimetal films was considered by Keldysh [15]. Boichuk et al. [16–19] calculated the effect of charge polarization on the energy of electrons of bivalent impurity and optical properties in spherical quantum dot. The effects of electric field and dielectric mismatch on physical properties in quantum dot are also calculated by Niculescu and Cristea [20]. The effect of dielectric constant and magnetic field on binding energy in cylindrical quantum wire is considered by Karki et al. [21].

The electronics properties of quantum structures confined in other nano-structures have attracted many researchers for their experimental applications. The study of impurity binding energy of a multilayered spherical GaAs/(Ga,Al)As quantum dot by Aktas and Boz [22], three dielectric layer models for the interface between a spherical quantum dot and the surrounding matrix by Deng [23], the binding energy of an impurity located at the center of multilayered quantum dot by Boz et al. [24] and the effect of dielectric-constant mismatch and magnetic field in multilayered SQD by Manaselyan and Kirakosyan [25] are a few examples of some interesting investigations in this field.

In this paper the binding energy of hydrogenic impurity located at the center of a GaAs ellipsoid with GaAlAs coating in the AlAs environment surrounding the system is calculated. In this regard, the interaction of electron with the polarization charges (which are caused by the impurity ion) and also self-interaction potential (due to the interaction of electron and its induced polarization charges) are taken into account. The outline of the paper is as follows: in Section 2 the Schrödinger equation solved for a hydrogenic impurity in an ellipsoidal quantum dot confined in the other EQDs, held at a finite potential, and the ground state energy and the wave function are calculated by applying the boundary conditions at the interfaces, then using the Ritz variational method, the impurity binding energy is calculated. Section 3 contains our results and discussion. Finally, the conclusions are presented in Section 4.

2. Theory

In the effective mass approximation, the Hamiltonian of an electron in each region of double ellipsoidal quantum dots in the presence of hydrogenic donor impurity can be written as

$$H_i=\frac{-\hbar^2}{2m_i^*}\Delta_R+U_i(R)+V_i(R)+W_i \quad (i=1,2,3) \tag{1}$$

where m_i^*, $U_i(R)$, $V_i(R)$, and W_i are the position-dependent effective mass, the confinement potential, the Coulomb potential and the self-polarization potential, respectively. For an EQD with circular cross-section in the X- and Y -plane the ellipticity constant is

$$\beta=1-\frac{c}{a} \tag{2}$$

where a and c are the semi-axes of the ellipsoid. It is useful to change the variables as follows [26]:

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

This change transforms the ellipsoid into a sphere of radius r_0, with the same volume. After these coordinate transformations the Hamiltonian can be represented as

$$H_i=H_{0i}+H_{1i}+W(r)+\Delta U(r) \tag{4}$$

where

$$H_{0i}=\frac{p^2}{2m_i^*}+U_i(r)+A_i. \tag{5}$$

A_i is the effect of the polarization charges induced on the quantum dot surface due to impurity ion, and is achieved by the electrostatic image method:

$$A_1=\frac{-e^2(\varepsilon_1-\varepsilon_2)}{r_{01}\varepsilon_1\varepsilon_2}+A_2,\quad A_2=\frac{-e^2(\varepsilon_2-\varepsilon_3)}{r_{02}\varepsilon_2\varepsilon_3},\quad A_3=0 \tag{6}$$

where r_{01} and r_{02} are the radii of double sphere and ε_i is the dielectric constant of different regions of dot. The confining potential $U_i(r)$ can be written as

$$U(r)=\begin{cases}U_1=0, & r\le r_{01}\\ U_2, & r_{01}<r<r_{02}\\ U_3, & r>r_{02}\end{cases} \tag{7}$$

The last term on the right-hand-side of Eq. (4), the non-spherical part of confinement potential, can be neglected [26]. For small ellipticity, $\beta>1$, the eigenvalues of the system can be determined using the variational method with H_{1i} as

$$H_{1i}=-\frac{e^2}{\varepsilon_i r}-\frac{\beta e^2}{3\varepsilon_i r}(1-3\ \cos^2\theta)+\frac{\beta}{3\ m_i^*}(\hat{p}^2-3\hat{p_z}^2) \tag{8}$$

The electron will also induce polarization charges at the boundary. $W(r)$ in Eq. (4) is the electron self-polarization potential which originates from the interaction between the electron and its self-image [18]. The $W(r)$ is the solution of Poisson equation and can be written in terms of Green's function (G) [19]:

$$W(r)=-\frac{2\pi e^2}{\varepsilon(r)}\Delta G \tag{9}$$

where

$$\varepsilon(r)=\frac{\varepsilon_1+\varepsilon_2+\varepsilon_3}{2}\left\{1-\left(\gamma_1\tanh\left(\frac{r-r_{01}}{L_1}\right)+\gamma_2\ \tanh\left(\frac{r-r_{01}}{L_1}\right)\tanh\left(\frac{r-r_{02}}{L_2}\right)-\gamma_2\ \tanh\left(\frac{r-r_{02}}{L_2}\right)\right)\right\} \tag{10}$$

L_i is the thickness of transition layer between regions i and $i+1$, and $\gamma_i=\varepsilon_i/(\sum_{i=1}^{n}\varepsilon_i)$. The wave function of H_{0i} can be written as

$$\psi_{nl}(r,\theta)=R_{nl}(r)P_l(\theta) \tag{11}$$

where $R_{nl}(r)$ and $P_l(\theta)$ are the radial and angular parts of wave function respectively. The radial part of Schrödinger equation is exactly solvable and the solutions are Bessel functions:

$$R_i(r)=N_{1i}J_l(C_ir)+N_{2i}N_l(C_ir), \tag{12}$$

where N_{1i} and N_{2i} are normalization constants, and $C_i=\sqrt{(2m_i^*/\hbar^2)(E^0-U_i-A_i)}$. The angular part of the wave function is

$$P_l(\theta)=B_{1l}\ \sin(\sqrt{l(l+1)}\theta)+B_{2l}\ \cos(\sqrt{l(l+1)}\theta). \tag{13}$$

To calculate the eigenvalues of unperturbed part of the Hamiltonian, E_0, we use the continuity of wave function and its derivative at the boundary surface. The ground state energy for H is obtained by the variational method:

$$E=\min_{\lambda}\frac{\langle\phi|H|\phi\rangle}{\langle\phi|\phi\rangle} \tag{14}$$

where the wave function, $\phi=\psi_0(r,\theta)e^{-\lambda r}$, and λ is the variational parameter.

The binding energy is given as

$$E_b=E_0-E \tag{15}$$

where E_0 is energy of system without impurity.