Confinement effects on quasi 0D dimensional structure with $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ quantum wells

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Abstract. In this work we study the effects of barrier height and position on symmetric $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ quantum wells in absence of external influences. We use a variational method within the effective mass approximation to observe the effects on the structure. The donor trial function is taken as a product of the ground state wave function, with an arbitrary correlation function that depends only on ion-electron separation. It has been observed two peaks in the curves for the dependence of the ground-state binding energies versus the donor distance from the axis and it is shown that the impurity binding energy depends strongly on the impurity position, potential shape on both quantum wells.

1. Introduction

Quantum dots (QDs) have attracted huge attention due to their potential applications in solar cells [1], biomedicine [2], photo-detectors [3], quantum cascade lasers [4], single-photon sources [5, 6], and quantum computing [7]. It has been found out that the electronic and optical properties of QDs are extremely sensitive to size, stoichiometry, and shape which leads to a tunable absorption, emission, and polarization-sensitive-spectra [8]-[10]. This dependence comes from relatively small number of atoms forming such structures. In this work, we propose a simple variational method to analyze the on- and off-center D^0 ground states in which the problem of the donors confined in quasi 0D structure is reduced to the similar one for the hydrogenic analogous in an isotropic space [11]. Taking advantage of the high symmetry in the spherical quantum dots (SQDs) we apply this method to analyze the ground state binding energy as a function of the donor impurity position in the SQD with two quantum well considering different confinement potential height and barrier position.

2. Theoretical Formalism

Within the framework of the effective-mass theory, the dimensionless Hamiltonian in a system of reference $\mathbf{r}' = \mathbf{r} + \boldsymbol{\zeta}$ for a D^0 in a SQD, can be written as [12]:

$$\hat{H}(\mathbf{r}+\boldsymbol{\zeta}, Z) = -\nabla^2 + V(|\mathbf{r}+\boldsymbol{\zeta}|) - \frac{2Z}{r} \tag{1}$$

where the Z parameter is zero for the electron and one for the donor; $\boldsymbol{\zeta}$ and $\mathbf{r}$ designate the 3D-vectors of the ion and electron positions, respectively measured from the center of the structure and $V(r)$ is an arbitrary confinement potential. The effective Bohr radius $a_0^* = \varepsilon\hbar^2/m^*e^2$ and the effective Rydberg, $R_y^* = e^2/2a_0^*$ have been taken as units of length and energy, respectively. A a function for the D^0 ground state, we consider the following trial function

$$\Psi_{D^0}(\mathbf{r}) = f_0(\mathbf{r}+\boldsymbol{\zeta})\Phi_{D^0(r)} \tag{2}$$

Here, $f_0(\mathbf{r}+\boldsymbol{\zeta})$ is the ground state wave function for a free electron in the SQD and the envelope function $\Phi_{D^0(r)}$ depends only the electron-ion separation.

Starting from the variational principle of Schrödinger and using the procedure of the functional derivative developed by us [12] we obtain the following one-dimensional Euler-Lagrange equation for the function, $\Phi_{D^0(r)}$,

$$\frac{1}{J_0(r)}\frac{d}{dr}J_0(r)\frac{d\Phi(r)_{D^0}}{dr} - \frac{2}{r}\Phi(r)_{D^0} = [E_{D^0} - E_0]\Phi(r)_{D^0} \tag{3}$$

where the radial part of the Jacobian volume element $J(r)$ is related to the density of distribution $P(r)$ of the free electron charge over a sphere of the radius r as

$$J(r) = 4\pi r^2 P(r); P(r) = \frac{1}{2}\int_{-1}^{1} f_0^2(\sqrt{r^2+\zeta^2-2r\zeta x})dx \tag{4}$$

In our calculations, to find the D^0 energy, $E(D^0)$, we solve numerically the Eq. (3) by using the trigonometric sweep procedure [13]. Eq. (3) describes the hydrogen-like atom in an effective space with the radial part of the Jacobian volume element $J(r)$ [12].

For modeling a quantum dot containing two quantum wells,we use the empirical relationship $V_i(\rho) = 0.61[1.155x(\rho) + 0.37x^2(\rho)]eV$, to obtain the height of the potential barrier with the aluminum concentration as we can see in Eq. 5. Where $x(\rho)$ represents the aluminum concentration as a function of radial distance r. Thus the confinement potential given by the following expression:

$$V(\rho) = V_1\theta(-\rho,-R_1,W) + V_2\theta(-\rho,R_2,W) - V_3\theta(-\rho,R_3+W,W) + V_4\theta(\rho,R_4,W) \tag{5}$$

Where

$$\theta(z,z_0,W) = \begin{cases} 0; & z < z_0 - W \\ [(z-z_0)^2/W^2 - 1]^2; & z_0 - W \le z < z_0 \\ 1; & z \ge z_0 \end{cases} \tag{6}$$

$\theta(-\rho,-R_i,W)$ is soft-edge version of the Heaviside function R_i, V_i represent the radii and heights of the barriers,respectively; W is a parameter related to the width of the transition region. $W = 0.01a_0^*$ for rectangular barrier.

3. Results and Discussion

The Fig. 1 (left) shows the profile of the confinement potential with two wells (QW1 and QW2), finite height and rectangular shape. The internal and external potential remain unchanged $V_{int} = V_{ext} = 40R_y^*$ and only the potential used for the layer vary for values of the $V_{layer} = 10R_y^*, 20R_y^*, 30R_y^*$. The radii are $R_1 = 1a_0^*$,$R_2 = 2a_0^*$,$R_3 = 3a_0^*$ and $R_4 = 4a_0^*$, in consequence the layer width is $1a_0^*$. In Fig. 1 (right) we present the D_0 binding energy dependence on the donor displacement from the center of the $Al_{0.3}Ga_{0.7}As/GaAs/Al_{0.3}Ga_{0.7}As$ SQD with different values of V_{layer}.One can observe a successive displacement of the curve peaks

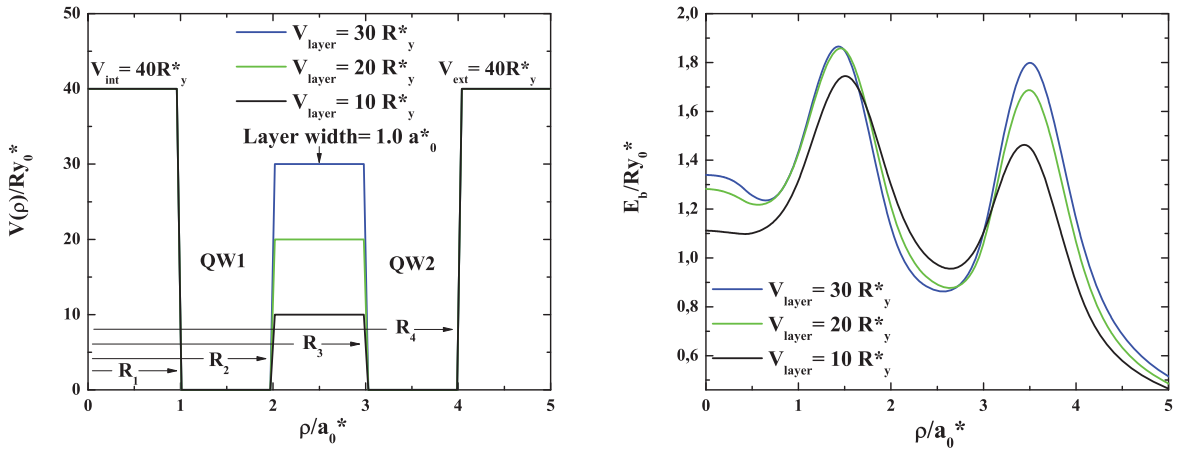

Figure 1. (left) Confinement potential profile containing two $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ quantum wells (QWs) and different values of V_{layer}. **Figure 1.** (right) D_0 ground state binding energies as a function of the donor displacement from the center of a spherical quantum dot.

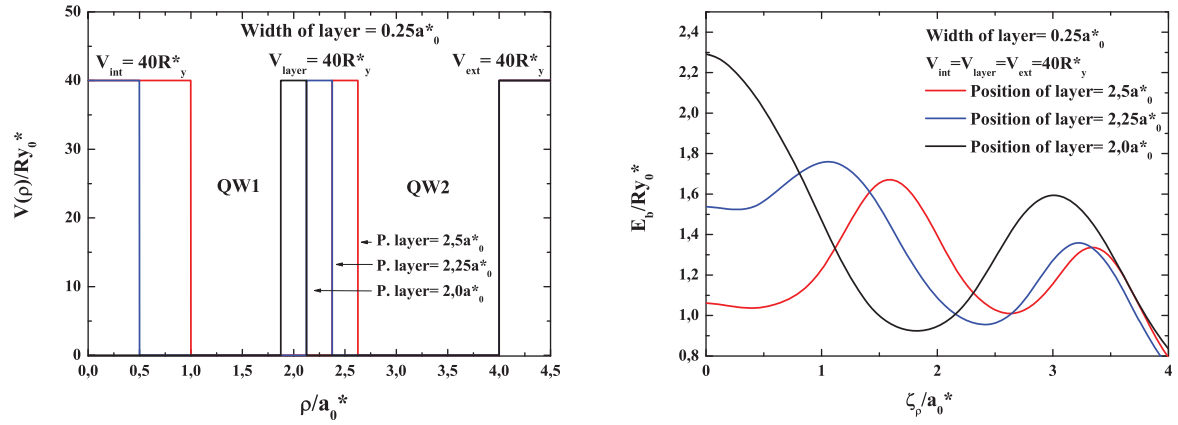

Figure 2. (left) Confinement potential profile containing two $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ quantum wells (QWs) and different values of layer position. **Figure 2.** (right) D_0 ground state binding energies as a function of the donor displacement from the center of a spherical quantum dot.

position to the layer with increase of the V_{layer} values, additionally the peaks are coinciding approximately with the midpoint between the interior and exterior radii, $(R_1 + R_2)/2$ for the firts peaks in QW1 whereas for the secund peaks are located approximately $(R_3 + R_4)/2$ in QW2, where the confinement is the largest. Moreover,the curves minimum in Fig. 1 are in the position of the layer, it shown that increasing V_{layer}, the probabilities of electron penetration in the barrier is reduced and he smallest value of the binding energy is achieved using $V_{layer} = 30R_y^*$, in additon, it is interesting that the crossovers of all curves related to the inversion of their order occur approximately at the same point, corresponding to distance at $2a_0^*$ and $3a_0^*$ from the axis of the SQD, in this position of the donor binding energy is almost

insensitive to the potential barrier changes. The Fig. 2 (left) also shows the profile of the confinement potential with similar characteristics than Fig. 1 (left), but the potential height are the same $V_{int} = V_{ext} = V_{layer} = 40R_y^*$, whereas the position of potential for the layer vary for values measured from the axis of the SQD $P.layer = 2.0a_0^*, 2.25a_0^*$ and $2.5a_0^*$ and the layer width is used $0.25a_0^*$. It is seen from Fig. 2 (right) that as the position layer is changed from $2.0a_0^*$ to $2.5a_0^*$ the altitude of the peaks in QW1 and QW2 falls as the P.layer increases. It is due to the fact that for those values, the electron mostly is localized in the central region of QW1 and QW2 and therefore, the electron-donor separation increases with the donor displacement from the dot center, whereas, the binding energy decreases when the donor is situated in the same position of the barriers, due to the electron-donor separation becomes very large. Additionally, the Fig.2 (right) shows a successive displacement of the curves peaks position to the right in the QW1 whereas the opposite occurs in QW2 with reducing P.layer in consequence a large curves configurations can be obtained.

4. Conclusions

In this paper, we have presented a simple method of calculation of the binding energy for the lowest states of the off-center D^0 donor in a SQD applicable for arbitrary confinement potential. By using this procedure we calculate the D^0 binding energies in dots with two rectangular wells with different values of potential barrier for the layer, in consequence, a large curves configurations can be obtained which is useful to design electronic and opto-electronic devices.

Acknowledgments

This work was partially financed by the Universidad del Magdalena (Fonciencias) and the Colombian Agency COLCIENCIAS through doctoral scholarships 567.

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