Impurity with two electrons in the spherical quantum dot with finite confinement potential

D A Baghdasaryan[1], **H Ts Ghaltaghchyan**[1], **E M Kazaryan**[1] **and H A Sarkisyan**[1,2,3*]

[1]Russian-Armenian (Slavonic) University, 0051 Yerevan, Armenia.
[2]Yerevan State University, 0025 Yerevan, Armenia,
[3]Peter the Great Saint-Petersburg Polytechnic University, St. Petersburg, 195251 Russia

*E-mail shayk@ysu.am

Abstract. Two-electron states in a spherical QD with the hydrogenic impurity located in the center and with a finite height confinement potential barrier are investigated. The effective mass mismatch have been taken into account. The dependence of ground state energy and Coulomb electron-electron interaction energy correction on the QD size is studied. The problem of the state exchange time control in QD is discussed, taking into account the spins of the electrons in the Russell-Saunders approximation. The effect of quantum emission has been shown.

1. Introduction

Electronic structure and optical properties of the semiconductor quantum dots (QDs) are of great interest in recent years [1] because of the rapid development of fabrication technology. Quantum dots QD or "artificial atoms" [1] have become the subject of the research during the last two decades. These systems can be considered as candidates in many technological applications, such as possible applications in memory chips [2], qubits in quantum computation [3,4], quantum cryptography [5], in room-temperature quantum-dot lasers [6], and photovoltaic elements based on quantum dots [7] and so on. The problem of theoretical study of two-electron and impurity states in 0-dimensional structures or quantum dots, quantum layers and rings has not only a purely academic but also an applied meaning.

The study of hydrogenic impurity states in semiconductor nanostructures was initiated through the work of Bastard [8]. After that, a number of theoretical investigations of hydrogenic impurity states in low dimensional semiconductors have been published [8-12].

In this paper, the two-electron states in a spherical QD with the hydrogenic impurity in the center with a finite height confinement potential barrier are investigated.

2. Theory

The Hamiltonian of the considered system is

$$\hat{H} = \sum_{i=1}^{2} \hat{H}_i + V(\vec{r}_1, \vec{r}_2), \tag{1}$$

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where $V(\vec{r}_1,\vec{r}_2)=\frac{e^2}{\varepsilon\left|\vec{r}_2-\vec{r}_1\right|}$ is the energy of interaction between the electrons, where ε – dielectric constant of QD material, and $\hat{H}_i$ – Hamiltonian of the one electron system which can be written as:

$$\hat{H}_i = T^{(i)} + V^{(i)}{}_{conf}(r_i) + V^{(i)}{}_{imp}(r_i). \tag{2}$$

Here $T^{(i)}$ is the kinetic energy of the electron, confining potential has the following form:

$$V_{conf}(r)=\begin{cases}-V_0, r<R\\ 0, r>R\end{cases}, \tag{3}$$

where R is the QD's radius. Potential of the impurity can be written as:

$$V_{imp}(r)=-\frac{Ze^2}{\varepsilon r}, \tag{4}$$

Where Ze is the impurity charge. In the current paper we are neglecting the dielectric constant mismatch of the QD and outer material taking into account the difference between effective masses of inner μ_1 and outer μ_2 materials.

Schrodinger equation in both inner and outer regions is spherically symmetric, so the one particle wave function will have following well-known form:

$$\Psi(r,\theta,\varphi)=\psi(r)Y_{l,m}(\theta,\varphi), \tag{5}$$

where $Y_{l,m}(\theta,\varphi)$ - spherical harmonics, l,m are orbital and azimuthal quantum numbers respectively, $\psi(r)$ is radial part of wave function. Substituting (5) in Schrodinger equation with Hamiltonian (2) and making notations $\rho=\frac{r}{a_B^*}$ where $a_B^*=\frac{\hbar^2\varepsilon}{\mu_1 e^2}$ – effective Bohr radius, $Ry=\frac{\mu_1 e^4}{2\hbar^2\varepsilon^2}$ effective Rydberg energy, and $\beta=\frac{\mu_1}{\mu_2}$.

In order to calculate ground state energy the variational method has been used. The trial function is taken in the form:

$$\psi_{tr}(\rho,\lambda)=\begin{cases}\psi^{(in)}{}_{tr}(\rho,\lambda), \rho<R\\ \psi^{(out)}{}_{tr}(\rho,\lambda), \rho>R\end{cases}, \tag{6}$$

$$\psi^{(in)}{}_{tr}(\rho,\lambda)=\exp\left(-\frac{\rho}{\lambda R}\right),\quad \psi^{(out)}{}_{tr}(\rho,\lambda)=C(\lambda)\exp\left(-\frac{\rho}{\lambda_{out}(\lambda)R}\right)$$

λ - is variational parameter. The dependence $\lambda_{out}(\lambda)$ is easy to find on the basis of the condition of continuity of the wave function at the point $\rho=R$ and BenDaniel -Duke condition.

$$\psi_{tr}^{(in)}(R)=\psi_{tr}^{(out)}(R),$$
$$\frac{1}{\mu_1}\psi'^{(\mathrm{in})}_{tr}(\rho=R)=\frac{1}{\mu_2}\psi'^{(out)}_{tr}(\rho=R), \tag{7}$$

From these conditions we get:

$$\lambda_{out}=\beta\lambda \tag{8}$$

Substituting (8) in the wave function continuity condition for $C(\lambda)$ we get:

$$C(\lambda)=\exp\left(\frac{\rho-\rho\beta}{R\beta\lambda}\right)$$

In the case when the mismatch of the effective mass is taken into account, Hamiltonian will have following form (for $\beta = 1$ we came to the case without effective mass mismatch):

$$\begin{cases} H_{in} = -\dfrac{d^2}{d\rho^2} - \dfrac{2}{\rho}\dfrac{d}{d\rho} + \dfrac{l(l+1)}{\rho^2} - \dfrac{2Z}{\rho} - V_0, \rho < R \\ H_{out} = -\beta\dfrac{d^2}{d\rho^2} - \dfrac{2\beta}{\rho}\dfrac{d}{d\rho} + \dfrac{\beta l(l+1)}{\rho^2} - \dfrac{2Z}{\rho}, \rho > R \end{cases} \tag{9}$$

In order to obtain ground state energy and variational parameter λ dependence on R we have to minimize the following integral:

$$I(\lambda, R) = \frac{\int_0^R \Psi_{tr}^{(in)} H_{in} \Psi_{tr}^{(in)} \rho^2 d\rho + \int_R^\infty \Psi_{tr}^{(\text{out})} H_{out} \Psi_{tr}^{(out)} \rho^2 d\rho}{\int_0^\infty |\Psi_{tr}|^2 \rho^2 d\rho} \to \min \tag{10}$$

Calculating the integral (10) we came to the following analytical expression:

$$\begin{aligned} I(\lambda, R) = \frac{1}{R^2\lambda^4} e^{-2/\lambda} (2 - 2\lambda + (\Lambda + e^{2/\lambda}\Lambda + 2R^2 V_0)\lambda^2 + \\ + 2R(RV_0 - e^{2/\lambda} Z)\lambda^3 - (e^{2/\lambda} - 1)R^2 V_0 \lambda^4 + \beta(-2 + 2\lambda + \Lambda\lambda^2)) \end{aligned} \tag{11}$$

where $\Lambda = -1 - 2l - 2l^2$.

We consider GaAs/GaAl$_x$As$_{1-x}$ quantum dot, thus the parameter β is equal to 0.73. From minimization condition (10) we obtain variational parameter dependence on the QD radius (Figure. 1).

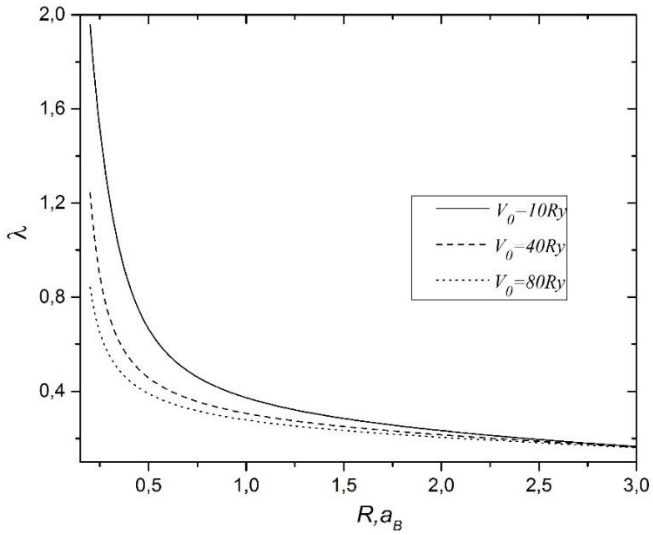


Figure 1. Variational parameter λ dependence on the QD radius at different V_0 (The case with effective mass mismatch, $Z = 2$).

Figure 1 shows the curve of the variational parameter λ behavior depending on the QD radius. Note that, for sufficiently large QD radii variational parameter asymptotically approaches $\lambda \to 1/R$. Which means that for infinitely large radii, the wave function is exactly equal to the Coulomb wave function of the bulk sample.

Let us calculate electron-electron interaction energy correction in the framework of the stationary perturbation method. Energy correction will have the following form:

$$\Delta V = \left\langle \Psi_{1s}(\rho) \middle| \widehat{V} \middle| \Psi_{1s}(\rho) \right\rangle, \tag{12}$$

Two-particle coordinate wave function, in the first approximation, can be written as the product of single electron functions. Taking into account spin of electrons in the Russell-Sounders approximation the two-electron wave function is the product of coordinate (triplet or singlet) and spin wave functions. Using calculation scheme, which has been considered in [14,15], for the energy correction, we come to the expression:

$$\Delta V(R) = \frac{e^2}{\varepsilon a_B} \int_0^{\infty} \int_0^{\rho_1} \psi^2\left(\lambda(R), \rho_1\right) \psi^2\left(\lambda(R), \rho_2\right) \rho_1 \rho_2^2 d\rho_2 d\rho_1 +$$
$$+ \frac{e^2}{\varepsilon a_B} \int_0^{\infty} \int_{\rho_1}^{\infty} \psi^2\left(\lambda(R), \rho_1\right) \psi^2\left(\lambda(R), \rho_2\right) \rho_1^2 \rho_2 d\rho_2 d\rho_1 \tag{13}$$

The results of integration of (13) are shown in Figure 2.

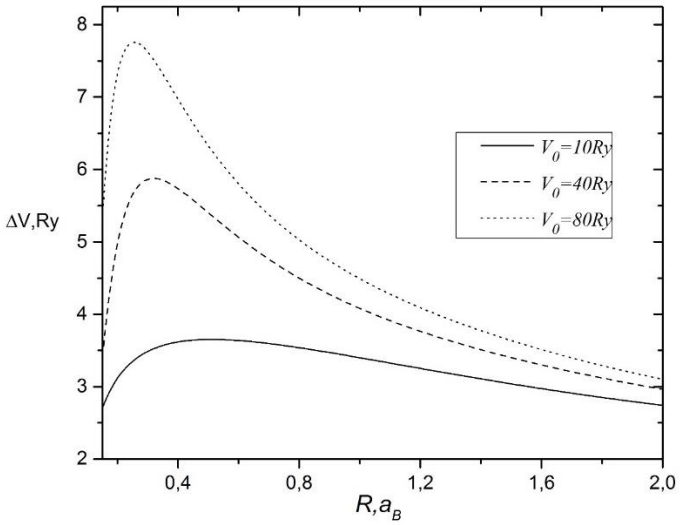


Figure 2. Energy correction dependence on the QD radius.

As we can see from Figure 2, there is an effect of quantum emission. The curve of energy correction dependence has a maximum, which corresponds to the radius at which quantum emission taking place (see Table 1). After the energy correction value decreases with the increase of quantum dot radius because electrons "feel" each other weakly. Using these results, we can calculate ground state energy of the two-electron system in the framework of perturbation theory (Figure 3):

$$E = 2E_0 + \Delta V, \tag{14}$$

where E_0 is the one-electron energy. ΔV - energy correction caused by electron interaction.

As can be seen from Figure 3 the energy of two-electron system monotonically decreases reducing from the positive region to the negative through zero with QD radius increase, because energy of size quantization decreases and full energy of the system monotonically reaches to energy of the bivalent donor impurity in the bulk sample. In the case when the electron-electron interaction is taken into account full energy of two-electron system can exceed the value of potential well depth V_0 Figure 4 shows that at a certain radius of the QD R_0 the energy of two electron system becomes equal to the depth of the potential well V_0. Therefore at radii less than R_0, one of electrons is emitted from the quantum dot. The value of QD radius at different depth of the potential well are presented in Table 1.

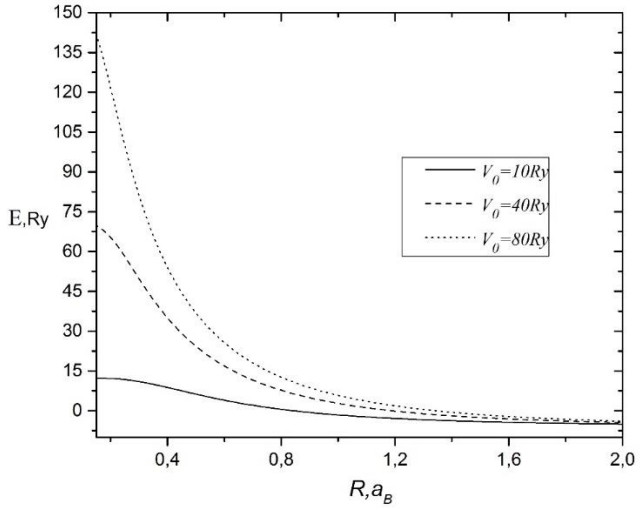


Figure 3. The dependence of the ground state energy of the system with electron-electron interaction on the QD radius.

Table 1. R_0 Dependence on the potential well depth V_0.

V_0,Ry	10	30	40	60	80
R_0, a_B	0.3489	0.3817	0.3626	0.3291	0.3032

The presence of the exchange integral, as mentioned in the introduction, leads to the exchange between the two states of the electrons [16]. They exchange their states for a time period (Figure 4):

$$\tau = \frac{\pi\hbar}{2A} = \frac{\pi\hbar}{2}\frac{1}{\Delta V}. \quad (15)$$

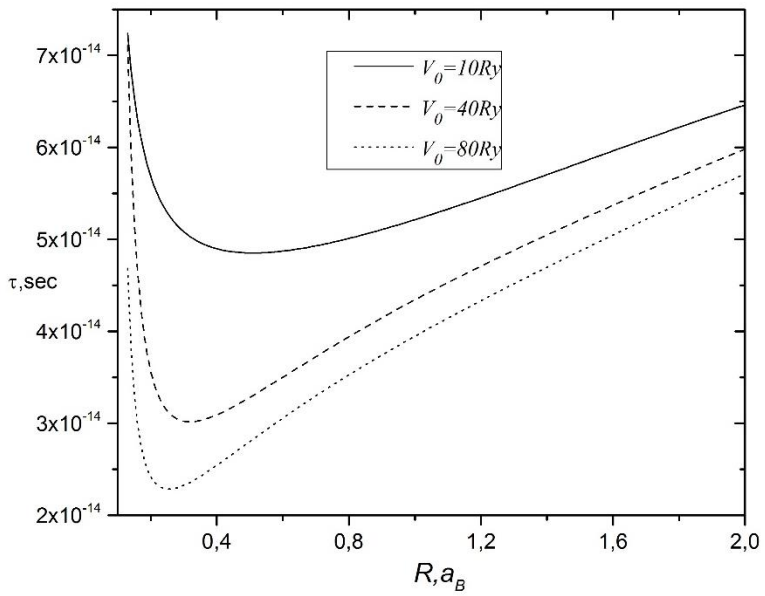


Figure 4. The dependence of the electrons state exchange time τ in the spherical quantum dot on the QD radius.

Figure 4 shows the electrons state exchange time dependence on QD radius. As we can see, the curves have minimum, which exactly corresponds to the value radii R_0 given in the Table 1.

3. Conclusion

Two-electron states in a spherical QD with the hydrogenic impurity located in the center with a finite height confinement potential barrier have been investigated. The dependence of ground state energy and Coulomb electron-electron interaction energy correction on the QD size is studied. The effect of effective mass mismatch have been studied. The state exchange time dependence on QD radius have been calculated.

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