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Electric Field Effect on Excited State Binding Energy and Self-Polarization of a Hydrogenic Impurity in a Spherical Quantum Dot

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ABSTRACT: Effects of the electric field and impurity position on the 2p-excited state self-polarization and binding energy of the electron-impurity in a spherical quantum dot are investigated as a function of the dot radius using variational approach. According to results, turning point of 2p-excited state binding energy changes with the electric field strength and position of impurity in the spherical quantum dot. Self-polarization and binding energy between the 1s-ground state and 2p-excited state of a hydrogenic donor impurity in SQD are presented as a function of the dot radius for different electric field value and impurity positions. Obtained numerical results show a good agreement with the literature.

Keywords: Self-polarization, turning point, spherical dot, binding energy, electric field.

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INTRODUCTION

In the last decades, low dimensional structures (LDS) have attracted great interest because of their potential application to high performance (Bastard, 1981; Greene and Bajaj, 1985; Brown and Spector, 1986; Fraizzoli et al., 1990; Zhu et al., 1990; Montenegro and Merchancano, 1992; Branis et al., 1993; Johnson, 1995; Tsaousidou and Butcher, 1997; Brandi et al., 2002 Mese and Okan, 2004; Ulas et al., 2004; Esuanu et al., 2009; Baskoutas and Terzis, 2009). The main problems in LDS are conductivity of semiconductor and optical properties. The impurities play an important role in LDS because optical and electronic properties will be controlled. In some recent theoretical studies concern with different shape and different confinement potentials have shown that binding energy depends on the impurity positions (Chuu et al.,1992; Sucu et al., 2008; Sadeghi, 2009; Özmen, et al., 2009; Hassanabadi and Rajabi, 2009; Sadeghi and Rezaie, 2010; Rezaei et al., 2012; Sivakami and Gayathri, 2013; Kang et al., 2013; Wang et al., 2014). Spherical quantum dot (SQD) is very important because of its high symmetry which simplifies the theoretical calculations. It is noticed that recent theoretical studies have concentrated on the self-polarization and ground state binding energy. Self-polarization is defined as effect of confining potential on the donor impurity (Okan et al., 2004; Ulas et al., 2005; Erdogan et al., 2006; Erdogan et al., 2006; Akankan et al., 2006; Tangarife and Duque, 2011; Erdogan et al., 2013). However, there are no studies on the calculation of the 2p-state self-polarization depends on the different impurity positions in a GaAs/AlAs SQD under electric field.

In this work, self-polarization and binding energy between the 1s-ground state and 2p-excited state of a hydrogenic donor impurity in SQD are presented as a function of the dot radius for different electric field value and impurity positions using variational approach.

MATERIALS AND METHODS

Hamiltonian for an electron under the electric field effect is defined as (Erdogan et al., 2013)

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + V(r) + eFr\cos\theta, \qquad (1)$$

m^* is the electron effective mass and $\vec{F}$ is electric field and applied along the z-axis. The confining potential is given by

$$V(r) = \begin{cases} 0 & 0 \le r \le R \\ \infty & r > R \end{cases} \qquad (2)$$

The ground state energy and wave-function within the spherical dot $(n = 1, l = 0)$ is obtained by solution of the Schrodinger equation (Erdogan et al., 2013),

$$\left[-\frac{\hbar^2}{2m^*}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right) + V(r) + eFr\cos\theta\right] R_{10}^0(r,\theta) = E_{10}^0 R_{10}^0(r,\theta), \qquad (3)$$

where upper subscript "0" refers to the subband. The eigenfunction, $R_{10}^0(r,\theta)$, and corresponding energy eigenvalue is given by (Ghazi et al., 2013; Bulut et al., 2014; Mese et al., 2017),

$$R_{10}^0(r,\theta) = \begin{cases} N_{10}^0 \frac{\sin(\alpha r)}{r} e^{-\beta r\cos\theta} & 0 \le r \le R \\ 0 & r > R \end{cases} \qquad (4)$$

$\alpha = \sqrt{2m^* E_{10}^0/\hbar^2}$ and where ground state energy E_{10}^0 determined by minimization of the variational parameter β.

In the presence of impurity, the 2p-state energy of conduction subband of system is obtained by solving the Hamiltonian is given by,

$$\left\{-\frac{\hbar^2}{2m^*}\left[\frac{\partial^2}{\partial r^2}+\frac{2}{r}\frac{\partial}{\partial r}+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right]+V(r)+eFr\cos\theta-\frac{e^2}{4\pi\varepsilon\varepsilon_0|\vec{r}-\vec{r}_i|}\right\}\Psi_{21}(r,\theta)=E_{21}(r,\theta)\Psi_{21}(r,\theta) \quad (5)$$

The 2p-state impurity energy $E_{21}(r,\theta)$ is calculated by variational approach. The trial wave function can be defined as (Villamil and Montenegro, 1999; Villamil et al., 2005; Bulut et al., 2014; Mese et al., 2017),

$$\Psi_{21}(r,\theta)=\begin{cases} N_{21}\frac{\sin(\alpha r)}{r}\, r\cos\theta e^{-\beta r\cos\theta}\, e^{-\lambda|\vec{r}-\vec{r}_i|} & r<R \\ 0 & r\geq R \end{cases} \quad (6)$$

where, r_i , N_{21} ,β and λ are impurity position which is along the z direction, normalization constant of 2p-excited state wave function and variational terms to include electric field and coulomb interaction, respectively.

The 2p-state binding energy is given by with difference of 1s ground state and 2p-excited state energy which defined as (Bulut et al., 2014),

$$E_b(r,\theta)=E_{10}^0(r,\theta)_{\beta_{min}}-E_{21}(r,\theta)_{(\lambda,\beta)_{min}} \quad (7)$$

where, $E_{21}(r,\theta)_{(\lambda,\beta)_{min}}$ 2p-state impurity energy determined by minimization of the variational parameters λ,β. (Sadeghi, 2009)

The self-polarization along the $\vec{r}_i$ direction for the 2p-state can be defined as (Okan et al., 2004)

$$\frac{SP}{e}=\frac{\langle\Psi_{21}(r,\theta)||\vec{r}-\vec{r}_i||\Psi_{21}(r,\theta)\rangle}{\langle\Psi_{21}(r,\theta)|\Psi_{21}(r,\theta)\rangle}-\frac{\langle\Psi(r,\theta)||\vec{r}-\vec{r}_i||\Psi(r,\theta)\rangle}{\langle\Psi(r,\theta)|\Psi(r,\theta)\rangle} \quad (9)$$

$\Psi(r,\theta)$ indicates the wave function in the absence of SQD and defined as (Erdogan et al., 2013),

$$\Psi(r,\theta)=Ne^{-|\vec{r}-\vec{r}_i|/2a^*}r\cos\theta \quad (10)$$

RESULTS AND DISCUSSION

In this section, the 2p-state binding energy(EB), the 2p-state binging energy turning point (TP) and 2p-state self-polarization for various impurity position in the GaAs/AlAs SQD is calculated. The parameters used in this paper are; m^*=0.067m_0, effective Bohr radius $a^* \cong 100\,A^0$,$\varepsilon = 12.26$ and Rydgerg energy $R^* = 5.83\,meV$. The results are presented in Fig.1-4.

In Fig. 1, the (BE) variation versus the dot radius for electric field strengths F= (0, 5 and 10) kV/cm in a SQD is presented. The results for the (TP) are in good agreement with F=0 kV/cm that reported

(Bulut et al., 2014). As seen from the Fig.1 that the (BE) becomes negative at the different dot radius depends on electric filed which means that 2p-state unbounded. It means that, the 2p impurity energy E_{21} is higher than the 1s ground state energy E_{10}^{0} with regard to our definition of binding energy. The (TP) is defined as the value of dot radius where the (EB) changes from negative to positive. It seen from the Fig.1 that the (BE) becomes positive at radius values greater than 2.72a* for F=0 kV/cm and r_i=0. Also, it can be seen that this result is in agreement with Refs. (Sadeghi and Rezaie, 2010). The small difference is due to the finite potential barrier. While the electric field strengths increase the (TP) shifts toward smaller dot radius. The turning point values for the electric field strengths F= (5 and F=10) kV/cm have found as 2.29a* and 2.02a*, respectively. As seen Fig.1, Increasing the electric field strengths increases the positive (EB). It is quite the opposite according to the 1s ground state.

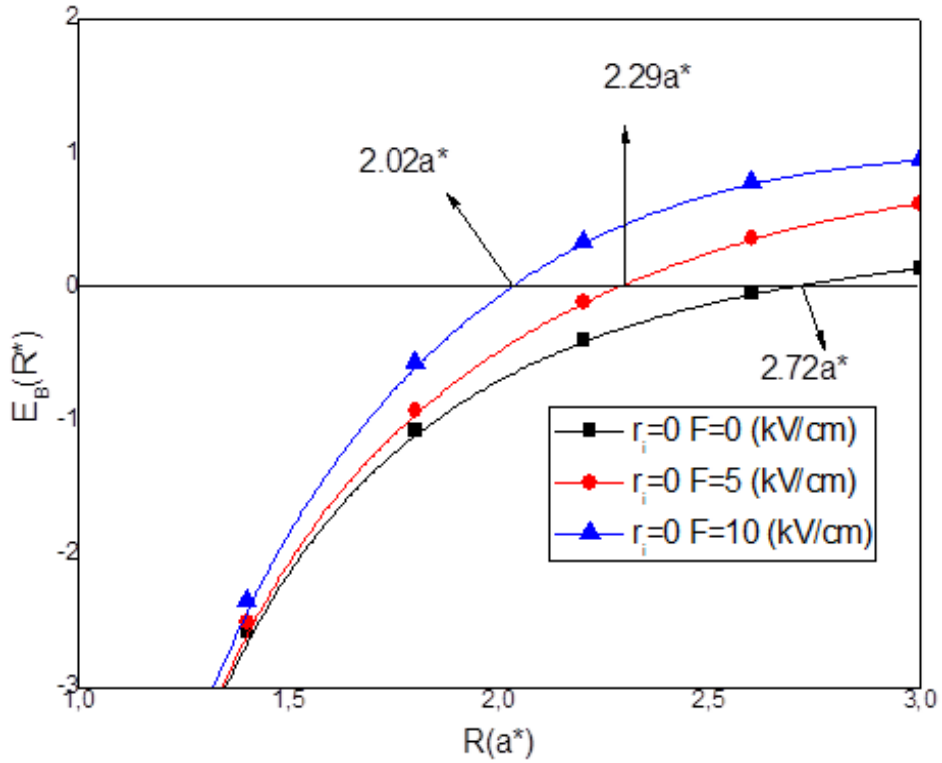

Figure 1. The 2p-state binding energy versus the dot radius for the electric field strengths F=(0, 5 and 10) kV/cm at impurity position r_i=0.

Fig. 2 depicts 2p-state self-polarization versus the dot radius for different electric field strengths. It is seen that the 2p-state self-polarization linearly increases with the electric field strengths. This is due to the fact that the growth of the electric field strengths reduces the potential of confinement and extends the areas of the wave function. As a result, self-polarization increases. This result is compatible with previous calculations (Erdogan et al., 2006).

The (TP) versus the dot radius for different impurity positions (r_i=0, R/2 and R) and electric field strengths F= (0 and 10) kV/cm is presented in Fig.3. It is observed that (TP) decreases when the impurity shifts toward from centre to r_i=R/2 for F=0 kV/cm. On the other hand, (TP) increases when the impurity shifts toward from r_i=R/2 to edge of the quantum dot for electric field strength F=0 kV/cm. When the impurity shifts toward from centre to edge of the quantum dot for electric field strength F= 10 kV/cm the (TP) increases. It is observed that electric field strength is effective on the (TP) value. This is due to the additional confinement cause by the electric field.

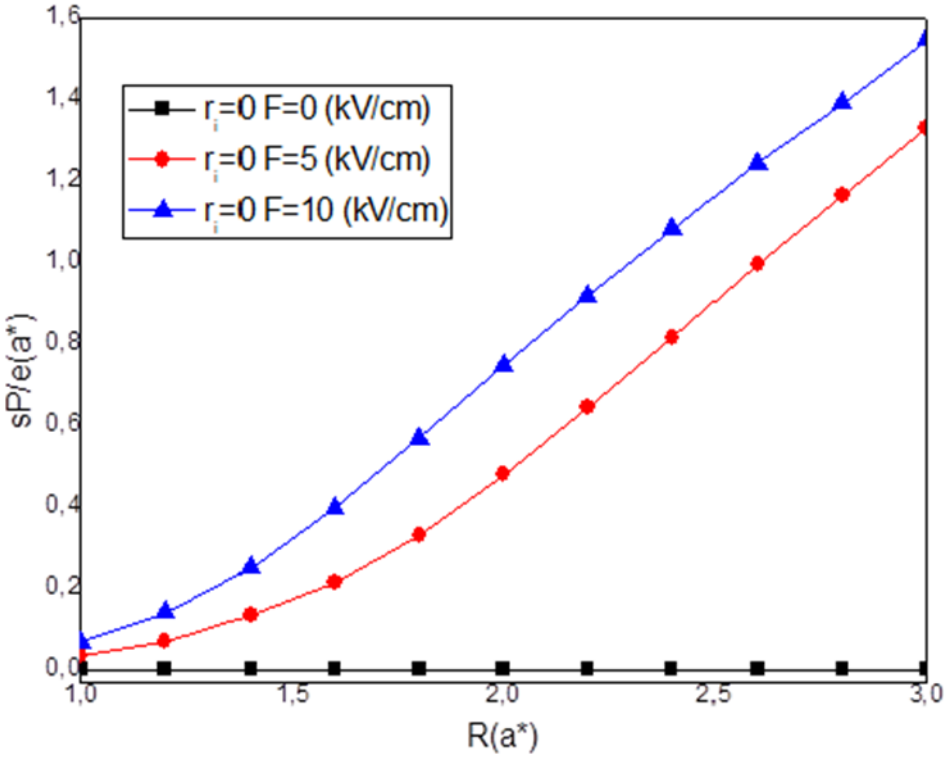

Figure 2. The 2p-state self-polarization as a function of dot radius for same electric field strengths and impurity position with Figure 1.

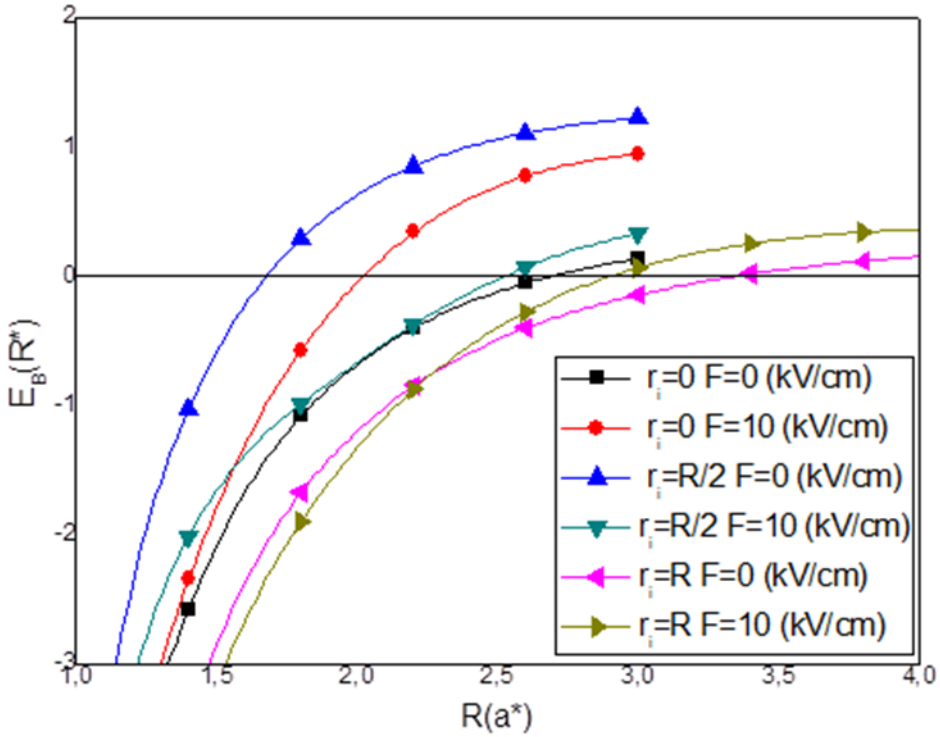

Figure 3. The 2p-state binding energy versus the dot radius for the electric field strengths F=(0 and 10) kV/cm and impurity positions r_i =0, r_i=R/2 and r_i=R.

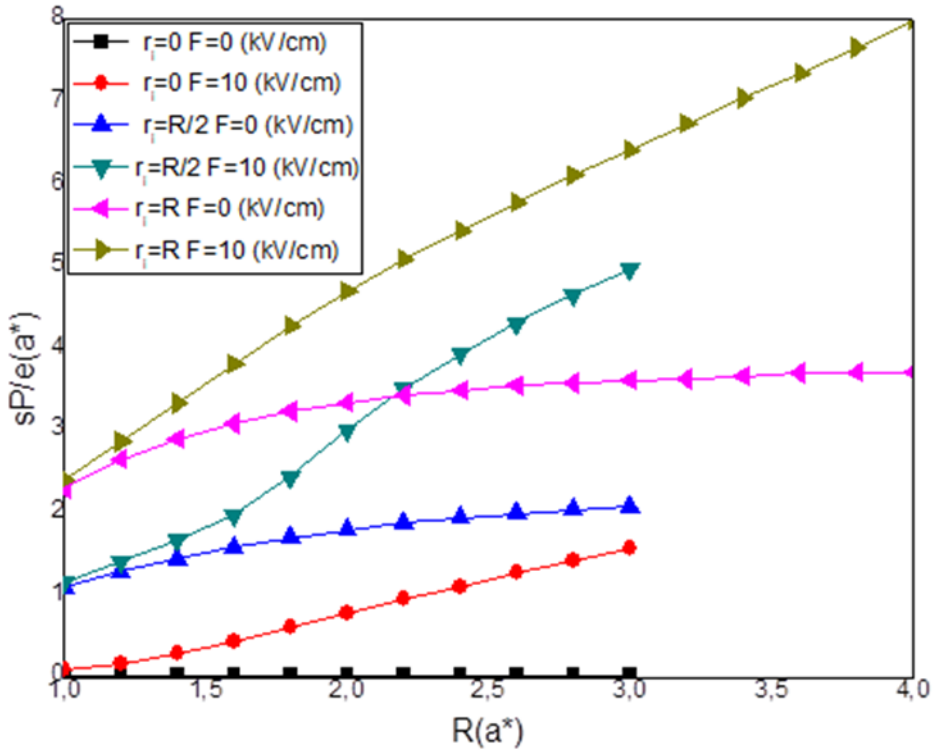

Figure 4. The 2p-state self-polarization versus dot radius for same electric field strengths and impurity positions with Figure 3.

To show the more effect of the impurity position on the 2p-state self-polarization, the 2p-state self-polarization versus the dot radius for different impurity positions (r_i=0, R/2 and R) and electric field strengths F= (0 and 10) kV/cm has plotted in Fig. 4. As seen from the Fig.4, when the impurity shifts toward from centre to edge of the quantum dot for electric field strengths F= (0 and 10) kV/cm, the 2p-state self-polarization approximately linearly increases. For very large quantum dots, the results tend towards to three-dimensional bulk case (Bulut et al., 2014; Mese et al., 2017).

CONCLUSION

The effects of impurity position and electric field strength on the (TP) versus dot radius are calculated. The results show that the effects of electric field and impurity position are very important on (TP). The first time 2p-state self-polarization in spherical quantum dot has been calculated.

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