

Electric field and concentration effects on the binding energy of a non - hydrogenic donor impurity in a finite cylindrical quantum well wire

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The effects of the electric field and concentration on the non-hydrogenic binding energy of a shallow donor impurity in a finite cylindrical quantum well wire (CQWW) of GaAs/ Al_xGa_{1-x}As was investigated. Within the effective mass approximation, we have calculated the non-hydrogenic binding energy of donor impurity by a variational method as a function of applied electric field, the wire radius, donor impurity positions and concentration of Al. We have investigated the concentration effect of Al on the non-hydrogenic binding energy as a function of electric field, wire radius and impurity position in QWW. It is shown that the difference in donor binding energy in the hydrogenic and non-hydrogenic regimes varies with radius of QWWs and impurity position while the interplay of the electric field is the same.

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1. Introduction

Low dimensional systems have revolutionized semiconductor physics. They rely on the technology of hetero-structures, where the composition of a semiconductor can be changed on the scale of nanometer. The energy levels are widely separated if the well is narrow and all electrons may be trapped in the lowest level. Motion parallel to the layers is not affected. However, so the electrons remain free in those directions.

The result is a two dimensional electron gas and the holes can be trapped in the same way [1]. In recent years, low dimensional semiconductor quantum wire systems have attracted a great deal of interest, both because of the possibility of investigating physical properties and their technological applications in electronic and optical devices [2,3]. The understanding of the electronic and optical properties of impurities in these systems is important. Theoretical and experimental studies of the effect of the confinement on the hydrogenic and non-hydrogenic impurity have been reported [4,5]. However, there are relatively few quantitative studies on quantum well wires (QWWs) in the presence of an external applied electric field [6,7].

There have been a number of studies of physical properties of shallow donor in quantum well wires [8-14]. For impurity states in quantum wires, the effects of several factors on impurity spectra have been investigated the shape of the wire's cross-section, the transverse dimensions of the wire, the height of the potential barriers, the position of the center with respect to the axis of the wire and the external applied electric and magnetic field. Most calculations have been performed for a

hydrogenic impurity in the effective mass approximation and within the variational approach: Electric fields have become an interesting probe for studying the physical properties of low dimensional systems, both from theoretical and technological point of view [15-19].

The physics of hydrogenic and non-hydrogenic impurities in QWWs under electric fields are also studied by number of authors [20-27]. Montes et al. [6,7] have presented the effect of an electric field and the geometric form of the system on the binding energy of shallow donor impurities in QWWs. Sukumar and Navaneethakrishnan studied the non-hydrogenic binding energy of shallow donor impurity in a square cross-sectional QWW, assuming the donor at the origin [28]. Csavinszky and Oyoko [29] have calculated the binding energy of on-axis hydrogenic and non-hydrogenic donors with zero electric field as a function of the radius of the QWW of circular cross-section, assuming the impurity located at the origin. Dalgic and co-worker have also studied the hydrogenic and non-hydrogenic binding energies of structure for infinite confinement potentials [25].

Recently, in our previous work [30], we have calculated the ground state binding energies of both hydrogenic and non-hydrogenic donor impurity located in different position of the square QWW with finite confining potential under applied electric field. We have also shown that the choice of the dielectric function is important, especially for small wire widths and the contribution from the dielectric screening to the binding energy is not significant for large wire widths.

In this work, we have investigated effects of electric field and Al concentration on the ground state binding energy of hydrogenic and non-hydrogenic donor impurity

in a cylindrical GaAs CQWW with finite confinement potential where electric field is applied parallel to the axis of the wire. Our results are given as a function of the wire radius, impurity positions for different electric fields and concentration of Al. We have also presented ΔE_b which is difference of binding energy between non-hydrogenic and hydrogenic case for different Al concentration. The calculations are made in the effective mass approximation within variational method, using a finite confining potential.

2. Theory

In the effective mass approximation, the Hamiltonian for the CQWW which lie along z -direction is

$$H_0 = -\frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} \right) + V(\rho, \phi) \quad (1)$$

where m^* is the electronic effective mass and $V(\rho, \phi)$ is the finite confinement potential given by

$$V(\rho, \phi) = \begin{cases} 0 & \rho \leq d \\ V_0 & \rho > d \end{cases} \quad (2)$$

The wave function for the ground state becomes

$$\Psi_0(\rho, \phi) = N_0 \begin{cases} J_0(r_{10}\rho) & \rho \leq d \\ \frac{J_0(r_{10}d)}{K_0(b_{10}d)} K_0(b_{10}\rho) & \rho > d \end{cases} \quad (3)$$

where N_0 is the normalization constant, the quantities $J_0(r_{10}\rho)$ is a Bessel Function of order zero and $K_0(b_{10}\rho)$ is a zero order modified Bessel Function. In Eq.(3) r_{10} and b_{10} are given by

$$r_{10} = \sqrt{\frac{2m^*E_0}{\hbar^2}} \quad b_{10} = \sqrt{\frac{2m^*(V_0 - E_0)}{\hbar^2}} \quad (4)$$

where E_0 is ground state energy. We calculate the effect of an electric field on the subband energies by using the Hamiltonian

$$H_1 = H_0 + \eta \rho \cos(\phi - \theta) \quad (5)$$

where $\eta = |e|F$ and F is the electric field strength applied perpendicular to axis of the wire. θ is the angle between the electric field and the positive x -axis. The trial function in this case is modified to be

$\Psi_1(\rho, \phi) = N_1 \Psi_0(\rho, \phi) \exp(-\beta \rho \cos(\phi - \theta))$ (6) where N_1 is the normalisation constant and β is the variational parameter. With an impurity at (ρ_i, θ) the Hamiltonian becomes

$$H_h = H_1 - \frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial z^2} \right) - \frac{e^2}{\epsilon \sqrt{z^2 + |\rho - \rho_i|^2}} \quad (7)$$

where h indicates the hydrogenic case and ϵ is the static dielectric constant. The trial wave function for the bound electron is defined as

$$\Psi_h = N_h \Psi_1(\rho, \phi) \exp(-\lambda_h \sqrt{z^2 + |\rho - \rho_i|^2}) \quad (8)$$

where N_h is the normalisation constant and λ_h is the variational parameter in the hydrogenic regime. For the non - hydrogenic donor the Hamiltonian is given by

$$H_{nh} = H_1 - \frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial z^2} \right) - \frac{e^2}{\epsilon(r) \sqrt{z^2 + |\rho - \rho_i|^2}} \quad (9)$$

where subscript nh indicates the non-hydrogenic regime and $\epsilon(r)$ is the Hermanson's spatial dielectric function [31], which can be expressed as

$$\frac{1}{\epsilon(\mathbf{r})} = \frac{1}{\epsilon} + \left(1 - \frac{1}{\epsilon} \right) \exp\left(-\frac{r}{c} \right) \quad (10)$$

where c is the screening constant. The trial wave function for the bound electron is taken to be

$$\Psi_{nh}(\rho, \phi, z) = N_{nh} \Psi_1(\rho, \phi) \exp(-\lambda_{nh} \sqrt{z^2 + |\rho - \rho_i|^2}) \quad (11)$$

where N_{nh} and λ_{nh} are the normalisation constant and the variational parameter in the non-hydrogenic regime, respectively. The binding energy of the non-hydrogenic impurity is defined as

$$E_b^{nh} = \left[\frac{\langle \Psi_1(\rho, \phi) | H_1 | \Psi_1(\rho, \phi) \rangle}{\langle \Psi_1(\rho, \phi) | \Psi_1(\rho, \phi) \rangle} \right]_{\rho_{min}} - \left[\frac{\langle \Psi_{nh}(\rho, \phi, z) | H_{nh} | \Psi_{nh}(\rho, \phi, z) \rangle}{\langle \Psi_{nh}(\rho, \phi, z) | \Psi_{nh}(\rho, \phi, z) \rangle} \right]_{\lambda_{nh_{min}}} \quad (12)$$

The hydrogenic binding energy can be obtained by replacing $\psi_h(x, y, z)$ placed in the right-hand side of equation (12) with $\psi_{nh}(x, y, z)$. Numerical results are found for the GaAs/Ga_{1-x}Al_xAs system where in the finite-barrier model we have taken $V_0 = 0.6(1.247x)$ eV, $\epsilon = 12.5(1-x) + 10.1x$ and x is concentration of Al.

3. Results and Discussion

We have presented impurity binding energies as a function of wire radius and impurity position in cylindrical quantum well wire under the different electric fields. Also we have presented impurity binding energies of hydrogenic and non-hydrogenic case as a function of Al concentration under the zero electric field. Finally, we have calculated difference of impurity binding energies as a function of wire radius for three different values of Al concentration. The values of physical parameters used in our calculations are reduced effective units of length and energy, which are given an effective Bohr radius

$$a^* = \hbar^2 \epsilon / m^* e^2 = 98.7 \text{ \AA}$$

$$R^* = e^2 / 2\epsilon a^* = 5.83 \text{ meV}$$

and effective mass $m^* = 0.067m_0$ (m_0 is free electron mass).

The behavior of the binding energy of hydrogenic and non-hydrogenic donors under zero electric field is presented in Fig. 1 as a function of the wire radius of CQWW for the impurity located at centre and $\rho_i = 0.5d$.

It is clear that binding energies in both regimes tend to finite values as the diameter of the wire tends to zero. It has found that the binding energies are almost equal at the large wire radius. However the discrepancy in the calculated binding energy for the impurity on-centre is greater than the impurity located at $0.5d$ in both regime. The binding energy difference becomes small as the impurity is located away from the centre. Thus screening effect is more pronounced for the small wire radius as $d \leq 1.25a^*$.

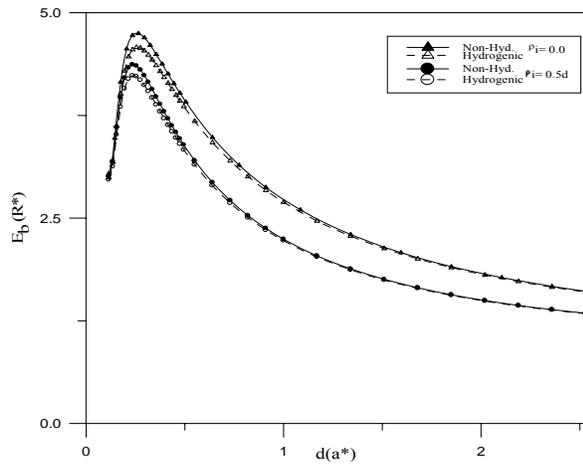


Fig. 1. Binding energy of donor impurity as a function of wire radius under zero electric field.

The binding energies as a function of the wire radius at the impurity located at the center and $\rho_i = 0.5a^*$ are shown in Fig. 2(a) and Fig. 2(b) for three different electric fields, respectively.

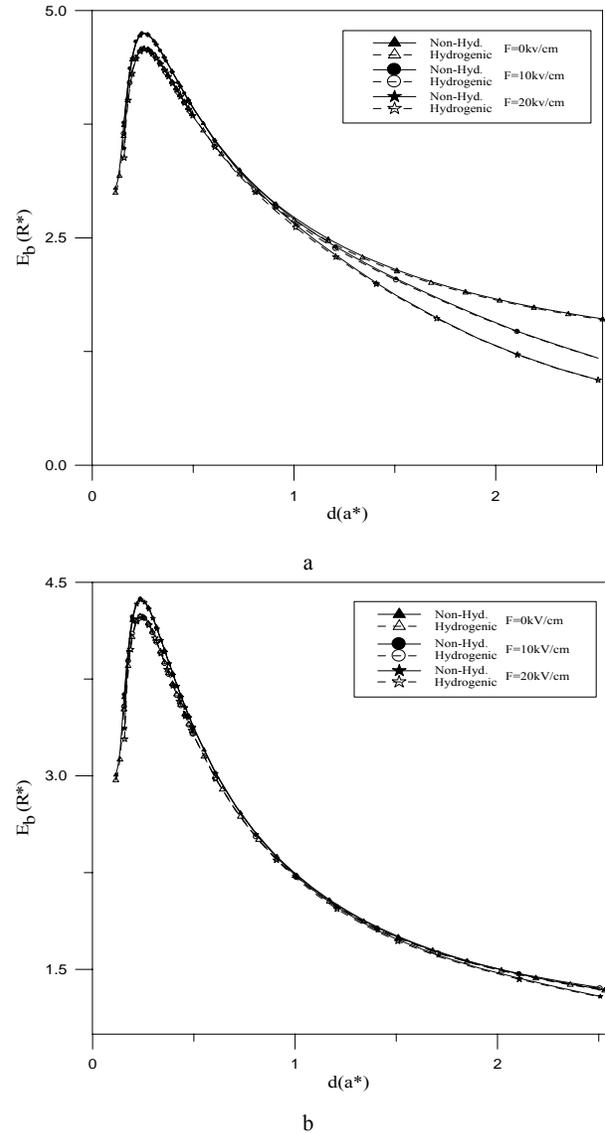


Fig. 2. Binding energies as a function of the wire radius under different electric fields at $x=0.3$. (a) impurity located at $\rho_i = 0.0$ and (b) impurity located at $\rho_i = 0.5d$.

The electric field is taken to be applied along the positive axis direction with $\theta = 0$. For both regimes, the binding energy is higher for smaller electric field strengths at both impurity positions given in Figs.2. It has found that there is no marked discrepancy in the hydrogenic and non-hydrogenic binding energies calculated with and without electric field when the wire radius is smaller than $d = 0.75a^*$. However the small changes in the electric field produce a large change in the binding energy at large wire radius for the impurity on-the centre. Thus, it can be mentioned that the binding energy in both regime more

sensitive to external electric field in the large wire radius where the impurity at the centre case.

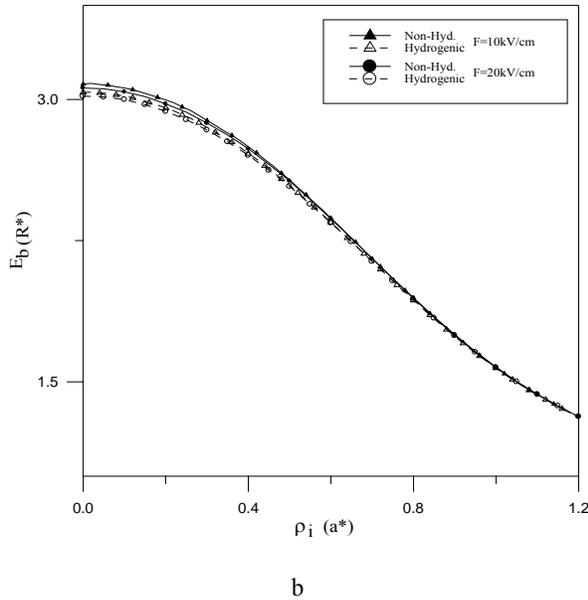
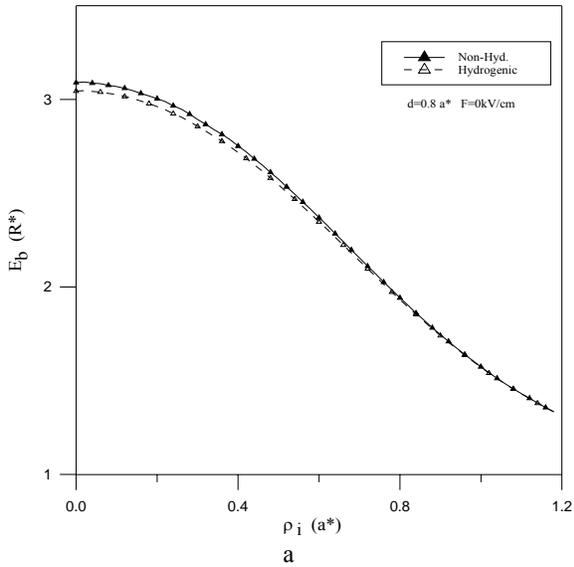


Fig. 3. Binding energies as a function of the impurity position along the wire radius $d = 0.8a^*$ at $x = 0.3$. (a) the electric field off and (b) different electric fields

Figs. 3(a) and 3(b) show the calculated binding energy as a function of the impurity position, which is located at different positions along the wire radius $d = 0.8a^*$ for the field off and field-on respectively. As it can be observed that, as expected for the hydrogenic case, the non-hydrogenic binding energy of the donor impurity under different applied electric fields decreases slowly as the impurity moves from the centre to the boundary of the

wire. It should be noted that the non-hydrogenic binding energy of the donor impurity under different electric fields behaves as in the hydrogenic case. As expected the hydrogenic regime, the applied electric field affects the binding energy decrease at all impurity positions. It has noted that the field off results for the hydrogenic case almost corresponds to the non-hydrogenic results for the impurity position up from approximately $0.7a^*$, but down from this value a small difference can be observed. This difference is due to the behavior of Hermanson's spatial dielectric function around the impurity position at the center.

The variation of the binding energy of donor impurity in two regimes displays as a function of Al concentration x with the wire radius $d = 1a^*$ at different impurity positions under zero electric field. Figure 4 shows the binding energy calculated in each regime increases equally with Al concentration increasing. The binding energy is higher for on the centre impurity than when the impurity is away from the centre of the wire for all Al concentrations. The concentration dependence of non-hydrogenic binding energy under zero electric field behaves as the hydrogenic case.

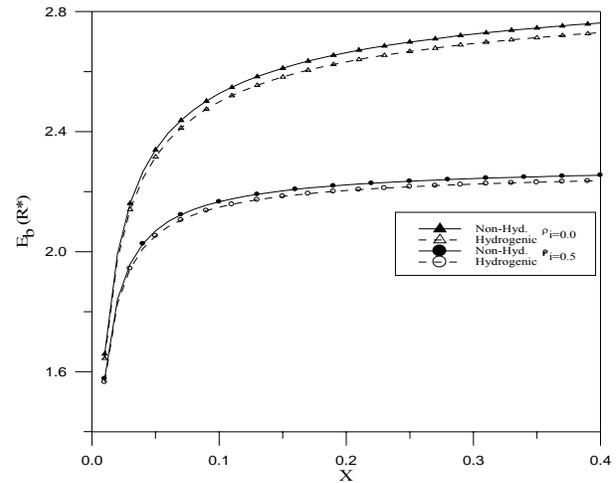


Fig. 4. The binding energy as a function of Al concentration x for hydrogenic and non-hydrogenic impurities with the wire radius $d = 1a^*$ at different impurity positions.

In order to get a clear picture of the screening effect on the binding energy of donor impurity we define the binding energy difference ΔE_b due to the effect of Hermanson's spatial dielectric function as the difference in two donor binding energies: $\Delta E_b = E_b^{nh} - E_b^h$.

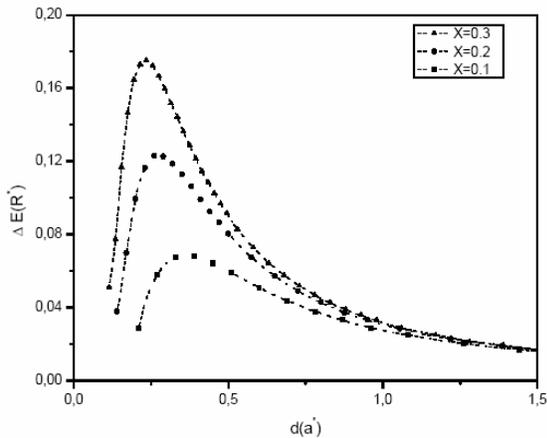


Fig. 5. The variation of binding energy difference ΔE_b as a function of the wire dimensions at different Al concentrations for the impurity located at centre and under zero electric field.

Fig. 5 shows this binding energy difference as a function of wire radius at three different Al concentrations for the impurity located at centre and under zero electric field. Note that ΔE_b shows the same behavior as the binding energy. ΔE_b increases more rapidly up to a maximum and then begins to decrease before reaching a constant value in larger wire radius. We can explain this behavior that the donor electron becomes close to the donor impurity ion, resulting in an increase in the binding energy. The maximum in the binding energy occurs close to $0.25d$ and $\rho_i = 0.0$, whereas for small Al concentration x values the position of the maximum peak is observed at large wire radius positions. There is no marked discrepancy for each Al concentration in the large wire radius of CQWW, as expected from the behavior of the Hermanson's spatial dielectric function which can be explained with Eq. (10). We should note that the binding energy difference decreases as the impurity moves from center to the edge of the wire. For the smaller distances $r \rightarrow 0$, $\varepsilon(r) \rightarrow 1$ and for the larger distances the screening is constant with $\varepsilon(r) \rightarrow \varepsilon$.

4. Conclusions

We have investigated impurity binding energy as a function of wire radius and impurity position under the applied electric field. Also we have studied the impurity binding energy depending on Al concentration in QWWs structures by using effective mass approximation in cylindrical coordinates. The results show that the binding energies of the non-hydrogenic donor impurity located outside of the centre wire are same influenced due to the

electric field with hydrogenic case. The effect of the Hermanson's spatial dielectric function is to increase the non-hydrogenic binding energy with decreasing widths compared to the hydrogenic case. We find that the difference in donor binding energy in two regimes is due to the dielectric function. By comparing the results for CQWW with that of a previous study [25], we conclude that, for the impurity located at the edge of the CQWW, the donor binding energy for small wire radius values in the finite and infinite confinement potentials are nearly the same. It is noted that the changes in the binding energy strongly depend not only on the quantum confinement but also on the impurity position on the electric strengths.

Finally, the results obtained in this work are capable of describing correctly the behavior of non-hydrogenic shallow donor impurities in CQWW under an applied external electric field. On the other hand, the results show that binding energy difference ΔE_b increases between non-hydrogenic and hydrogenic cases as Al concentration increases in the CQWW.

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