

ELECTRIC FIELD EFFECT ON THE BINDING ENERGY OF A NON-HYDROGENIC DONOR IMPURITY IN A SQUARE QUANTUM WELL WIRE

S. Dalgic*, M. Ulaş, B. Ozkapi

Department of Physics, Trakya University, 22030 Edirne, Turkey

We have used a variational technique to calculate the effect of an electric field on the non-hydrogenic binding energy of a donor impurity in a square GaAs/Ga_{1-x}Al_xAs quantum well wire (QWW). The non-hydrogenic binding energy of the donor impurity was calculated by the variational method as a function of applied electric field, the wire radius and donor impurity position. The results show that the non-hydrogenic binding energy of donor impurity located around the centre is larger than that of the hydrogenic binding energy. In this work, the variational method employed is capable of giving all the correct trends for impurity binding energies as a function of applied electric field, impurity position and screening effect.

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1. Introduction

In the last two decades low-dimensional heterostructure systems such as thin films, wires and quantum dots [1-2] have received a great deal of attention. However their interesting physical properties [3,4] and their technological applications in electronic and optical devices. In semiconductor materials, an applied electric field is a subject of fundamental interest for probing the physical properties of new device principle. The effect of applied electric on the binding energy has been the subject of insensitive investigation. The presence of hydrogenic impurities is one of the main problems in semiconductor low-dimensional systems, since the presence of the impurity states in the nanostructure affects both the electronic mobility and the optical properties. Much work has been devoted to the study of hydrogenic impurity states in these systems. Binding energy calculations for hydrogenic impurities in quantum wells (QWs) [5-7], quantum well wires (QWWs) [8-10] and quantum dots (QDs) [11-13] have been performed. It is found that when the dimensions of the system are reduced, the quantum size becomes clear and an effective strength of the Coulomb interaction increases. Thus the binding energy of the electron should be larger in lower dimensions.

The effect of an electric field on the hydrogenic binding energy was presented by several authors [14-21]. The effect of an electric field and the geometric form of the system on the binding energies of shallow donor impurities in QWWs was presented by Montes et al. [22-24] and Ulaş et al. [14,15]. They found that the hydrogenic binding energy of a shallow donor impurity is a rather sensitive function of the geometry of the QWW and of the distribution of impurities inside the QWW. Some theoretical work has been reported on the calculations for the non-hydrogenic binding energies of donor impurities in QWWs [24-27] taking into consideration the *r*-dependent dielectric response.

Sakumar and Navaneethakrishnan studied the non-hydrogenic binding energy of a shallow donor impurity in a square cross-sectional QWW, assuming the donor at the origin [28]. Their calculations were performed with two different dielectric functions, the first of which was previously used in the study of donor in the bulk of semiconductor systems as applied to QWWs. They have shown that the choice of the dielectric function is important, especially for small well widths and the contribution from the dielectric screening to the binding energy does not contribute significantly for larger well widths.

Csavinszky and Oyoko [29] have calculated the binding energies of on-axis hydrogenic and non-hydrogenic donors with zero electric field as a function of the radius of the GaAs-(Ga,Al)As

* Corresponding author: dseyfe@yahoo.co.uk

QWW of circular cross-section, assuming the impurity located at the origin. They have found that both hydrogenic and non-hydrogenic binding energies of donor impurities are sensitive functions of the QWW radius and, for infinite barrier height, increase as the radius decreases. Recently, Oyoko [30] has studied the effect of Hermanson's spatial dielectric function on the impurity binding energy in a cylindrical cross-sectional GaAs-(Ga,Al)As QWW under zero electric field. He concluded that this effect is to increase the binding energy of the non-hydrogenic donor impurity with decreasing radius over that of a hydrogenic donor.

To the best of our knowledge there are no theoretical studies considering the effects of applied electric fields on the binding energies of non-hydrogenic donor impurity located in different positions outside of the center of the square QWW with finite confining potential.

In the study we have calculated the ground state binding energies of both hydrogenic and non-hydrogenic donor impurity located in different positions of the square QWW with finite confining potential under applied electric field. The difference in donor binding energy in the two regimes, which is due to the effect of Hermanson's spatial dielectric function, has also been calculated as a function of the QWW width and impurity position. We have found that the binding energy for non-hydrogenic case is extremely sensitive to the impurity position. However the influence of the electric field for both binding energies is the same.

This paper is organized as follows. In Section 2, we present general formalism we deduce expression of the donor binding energies with electric field and the dielectric function. The numerical results and discussion are presented in Section 3. Finally, Section 4 summarizes the main results of the work along with a few concluding remarks.

2. Theory

It is convenient to use the Cartesian coordinates for wires of rectangular cross-section. The Hamiltonian for the wire of rectangular cross-section, lying along the z-direction, is

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

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

$$V(x, y) = \begin{cases} V_0 & x < -L_x/2 \quad ; \quad y < -L_y/2 \\ 0 & -L_x/2 \leq x \leq L_x/2 \quad ; \quad -L_y/2 \leq y \leq L_y/2 \\ V_0 & x > L_x/2 \quad ; \quad y > L_y/2 \end{cases} \quad (2)$$

Thus the electron is free to move along z-direction, but constrained along x- and y- direction. The subband structure of the wire is obtained by the variational method using the following trial wave function

$$\Psi_0(x, y) = N_0 \begin{cases} \exp(k_2(x+y)) & x < -L_x/2 \quad ; \quad y < -L_y/2 \\ \cos(k_1 x) \cos(k_1 y) & -L_x/2 \leq x \leq L_x/2 \quad ; \quad -L_y/2 \leq y \leq L_y/2 \\ \exp(-k_2(x+y)) & L_x/2 < x \quad ; \quad L_y/2 < y \end{cases} \quad (3)$$

where N_0 is the normalisation constant, $k_1 = \sqrt{2m^*E_0}/\hbar$, $k_2 = \sqrt{2m^*(V_0 - E_0)}/\hbar$. Matching the wave function and its derivative at the boundaries yields

$$k_2^2 = \frac{k_1^2(1 - \cos k_1 L)}{(1 + \cos k_1 L)} \quad (4)$$

We have taken the cross-section to be a square with sides $L_x = L_y = L$. Next, we calculate the effect of an electric field on the subband energies by using the Hamiltonian

$$H_1 = H_0 + \eta (x \cos \theta + y \sin \theta) \quad (5)$$

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

$$\Psi_1(x, y) = N_1 \Psi_0(x, y) \exp[-\beta (x \cos \theta + y \sin \theta)] \quad (6)$$

where N_1 is the normalisation constant and β is the variational parameter.

With an impurity at $(x_i, y_i, 0)$ the Hamiltonian becomes

$$H_h = H_1 - \frac{\hbar^2}{2m^*} \left(\frac{\partial^2}{\partial z^2} \right) - \frac{e^2}{\epsilon_0 \sqrt{|x - x_i|^2 + |y - y_i|^2 + z^2}} \quad (7)$$

where h indicates the hydrogenic case and ϵ_0 is the static dielectric constant. The trial wave function for the bound electron is defined as

$$\Psi_h(x, y, z) = N_h \Psi_1(x, y) \exp\left(-\lambda_h \sqrt{|x - x_i|^2 + |y - y_i|^2 + z^2}\right) \quad (8)$$

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

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

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

$$\frac{1}{\epsilon(r)} = \frac{1}{\epsilon_0} + \left(1 - \frac{1}{\epsilon_0}\right) \exp\left(-\frac{r}{c}\right) \quad (10)$$

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

$$\Psi_{nh}(x, y, z) = N_{nh} \Psi_1(x, y) \exp\left(-\lambda_{nh} \sqrt{|x - x_i|^2 + |y - y_i|^2 + z^2}\right) \quad (11)$$

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

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

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 $\hbar^2/m^*e^2 = 98.7 \text{ \AA}$ and x is concentration of Al.

3. Results and discussion

We have done a series of calculations and investigated the impurity binding energy as a function of electric field, wire width and impurity position. The calculations are carried out for the model system of GaAs/Ga_{1-x}Al_xAs for which we find the effective Bohr radius $a^* = \hbar^2 \epsilon_0 / m^* e^2 = 98.7 \text{ \AA}$ and effective Rydberg $R^* = e^2 / 2\epsilon_0 a^* = 5.83 \text{ meV}$.

The impurity binding energies of hydrogenic and non-hydrogenic cases in are shown in Fig.1 where we have calculated the binding energies as a function of length of square QWW for zero electric field our results perfect agreement with previous calculations without the electric field the binding energies are found to be almost identical for square cross-section if hydrogenic and non-hydrogenic cases are taken to be comparable.

The impurity position dependence of the binding energies is shown in Fig.2 where the impurity position is changed along the diagonal of the square wire ($L_i(a^*)$) without electric field. It can be seen that up from an impurity position of $0.08a^*$ the two binding energies decrease equally but from about $0.08a^*$ down a small difference can be observed. This difference is due to the behaviour of Hermanson's spatial dielectric function around the impurity position of the centre.

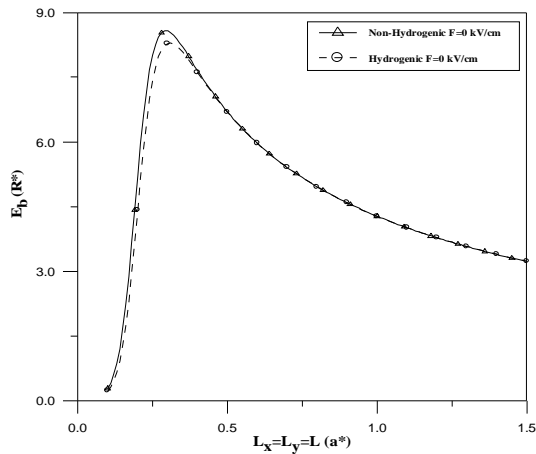


Fig. 1. The hydrogenic and non-hydrogenic binding energies as a function of side length of the square QWW without electric field.

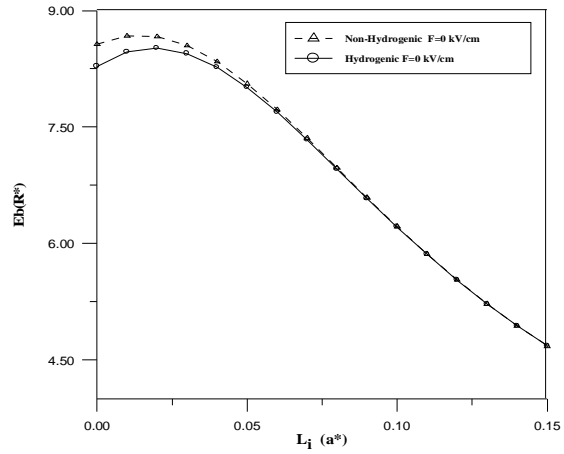


Fig. 2. The hydrogenic and non-hydrogenic binding energies as a function of impurity position of the square QWW without electric field.

The behaviour of the binding energies under different electric fields is shown in Fig.3 for square QWW. The impurity is taken to be at the centre of the wire. The electric field is taken to be applied along the positive axis direction with $\theta=0$. Thus, the electron shifts towards the negative part of the axis. It is seen from these figures that the hydrogenic and non-hydrogenic binding energies are a sensitive functions of the electric fields for square QWW. The non-hydrogenic binding energy under 10 kV/cm and 20 kV/cm electric fields are shown for comparison. They fit each other as well as hydrogenic binding energy. It should be note that in conventional symmetrical structures, the wave functions have a symmetrical structure and the wave functions have a symmetric character. So the donor impurity binding energy does not depend on the direction of the electric field. The energy becomes smaller when a field is applied for impurities located at outside of centre, as expected for hydrogenic case.

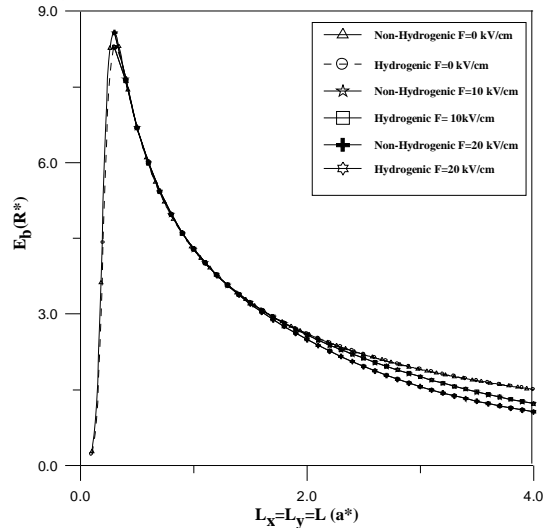


Fig. 3. The hydrogenic and non-hydrogenic binding energies as a function of side length of the square QWW for different electric field.

Fig. 4 shows the hydrogenic and non-hydrogenic binding energies as a function of the impurity position under different electric fields for square QWW. It can be seen that, as expected for the hydrogenic case, the non-hydrogenic binding energy of donor impurity under different applied electric fields decreases slowly as the impurity moves from the centre to the boundary of the QWW. It should be noted that the non-hydrogenic binding energy of the donor impurity under different electric fields behaves as in hydrogenic case. As expected the hydrogenic regime, the applied electric field affects the binding energy decrease at all impurity positions. The Al concentration, x , dependence of binding energy we show Fig.4. as expected increased the potential barrier increases the binding energy, because the electron is better pushed the Coulomb centre when the walls are at a higher potential

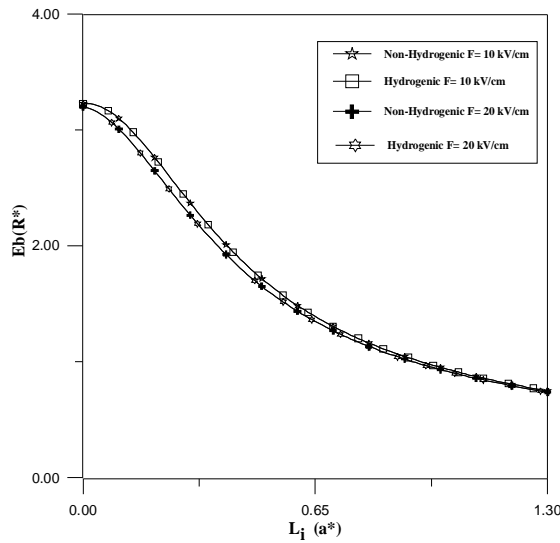


Fig. 4. The hydrogenic and non-hydrogenic binding energies as a function of impurity position of the square QWW for different electric field.

We have calculated the screening effect on the binding energies of donor impurity without electric field. We define the binding energies difference $\Delta E_b = E_b^{nh} - E_b^h$ which is the effect of Hermanson's spatial dielectric function. It is clear that the binding energies difference is more remarkable in the smaller dimensions of square QWW. We should note that for the smaller distances $r \rightarrow 0$, $\epsilon(r) = 1$ and for the larger distances the screening is constant with $\epsilon = 0.3$.

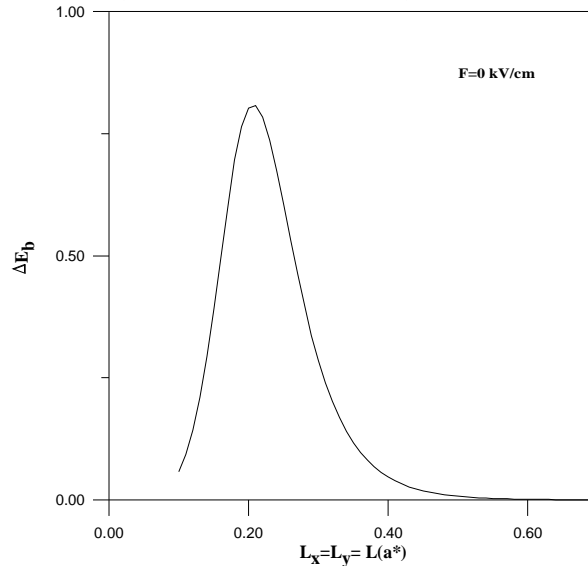


Fig. 5. The variation of binding energy difference as a function of the square QWW

4. Conclusions

In this study we have investigated the effect of an electrical field on the hydrogenic and non-hydrogenic binding energy of a shallow donor impurity located at different positions in square QWW's. We have used a variational method and within the effective mass approximation of the calculations. The changes binding energies depend not only the QWW width but also the applied electric field and impurity position in the QWW. In the two regimes the applied electric field produces an important effect on the impurity binding energies for the large well widths.

We have noted that the binding energy of the non-hydrogenic donor impurity located outside of the centre wire is influenced more due to the electrical field, as expected 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.

It is shown that the donor binding energy depends sensitively both on the external electric field and the position of the quantum well walls. In both cases, the binding energy increases as the electron pushed towards the Coulomb centre. Finally, the results obtained in this work are capable of describing correctly the behaviour of non-hydrogenic shallow donor impurities in square QWW's under an applied external electrical field.

References

- [1] W. Wegschneider, L. N. Pfeiffer, M. M. Dignam, A. Pinchuk, K. W. West, S. L. McCall, R. Hull, *Phys. Rev. Lett.* **71**, 4071 (1993).
- [2] H. Akiyama, T. Someya, H. Sakaki, *Phys. Rev.* **B53**, R10520 (1996); H. Akiyama, T. Someya, H. Sakaki, *Phys. Rev. B* **53**, R4229 (1996).
- [3] H. Sakaki, H. Noge (Eds.), *Nanostructures and Quantum Effects* (Springer, Heidelberg, 1993).
- [4] U.Woggon (Ed.), *Optical Properties of Semiconductor Quantum Dots* (Springer, Heidelberg, (1997).
- [5] G. Weber, *Appl. Phys. Lett.* **67**, 1447 (1995).
- [6] H. H. Hassan, N. El-Meshad, *Phys. Stat. Sol. (b)* **201**, 381 (1997).
- [7] J. Lee, H. P. Spector, *J. Appl. Phys.*, **57**, 366 (1985).
- [8] G. W. Bryant, *Phys. Rev. B* **29**, 6632 (1984); G. W. Bryant, *Phys. Rev.* **B31**, 7812 (1985).
- [9] J. A. Brum, *Solid State Commun.* **54**, 179 (1985).
- [10] J. W. Brown, H. N. Spector, *J. Appl. Phys.* **59**, 1179 (1986).
- [11] A. D. Yoffe, *Adv. Phys.* **42**, 173 (1993).
- [12] U. Waggon, S. V. Gaponenko, *Phys. Stat. Sol. (b)* **189**, 285 (1995).
- [13] C. Bose, *J. Appl. Phys.* **83**, 3098 (1998).
- [14] M. Ulas, H. Akbas, M. Tomak, *Phys. Stat. Sol. (b)* **200**, 67 (1997).
- [15] M. Ulas, E. Cicek, S. S. Dalgic, *Phys. Stat. Sol. (b)* **241**, 2968 (2004).
- [16] M. Ulas, I. Erdogan, E. Cicek, S. S. Dalgic, *Physica* **E25**, 515 (2005).
- [17] A. Puri, J. G. Sun, T. Odagaki, *Solid State Commun.* **70**, 907 (1989).
- [18] A. Montes, C. A. Duque, N. Porrás-Montenegro, *J. Phys.:Condens. Matter* **10**, 5351 (1998).
- [19] E. Kasapoglu, H.Sari, I. Sökmen, *Physica* **B315**, 261 (2002).
- [20] E. Kasapoglu, H.Sari, I. Sökmen, *Appl. Phys.* **A78**, 1053 (2004).
- [21] T. Kodama and Y. Osaka, *J. Phys. Soc. Japan* **55**, 3941 (1986).
- [22] A. Montes, C. A. Duque, N. Porrás-Montenegro, *Phys. Rev.* **B201**, 731 (1998).
- [23] A. Montes, C. A. Duque, N. Porrás-Montenegro, *J. Appl. Phys.* **84**, 1421 (1998).
- [24] A. Montes, C. A. Duque, N. Porrás-Montenegro, *J. Appl. Phys.* **81**, 7890 (1997).
- [25] N. Porrás-Montenegro, *J. Phys. Condens. Matter* **5**, A367 (1993).
- [26] V. Narayani, S. Sukumar, *Solid State Commun.* **90**, 575 (1994).
- [27] J. Hermanson, *Phys. Rev.* **B150**, 660 (1966).
- [28] B. Sukumar, K. Navaneethakrishnan, *Phys. Rev.* **B41**, 12911 (1990).
- [29] P. Csavinszky and H. Oyoko, *Phys. Rev.* **B43**, 9262 (1991).
- [30] H. Odhiambo Oyoko, *Ind. J. of Pure& Appl. Phys.* **38**, 512 (2000).