International Scientific Conference 20 UNITECH 26

INTERNATIONAL SCIENTIFIC CONFERENCE
19-21 November 2026
GABROVO

THE BINDING ENERGY IN ASYMMETRIC TRIPLE SQUARE QUANTUM WIRES UNDER AN ELECTRIC FIELD

F.K. BOZ[1*], A. BILEKKAYA[2], S. AKTAS[1], S.E. OKAN[1]

[1] Trakya University, Physics Department, 22030 Edirne, Turkey
[2]Trakya University, Edirne Vocational School of Technical Sciences, 22030 Edirne, Turkey

**Corresponding author: figenb@trakya.edu.tr*

Abstract

The effects of electric field on the binding energy of a hydrogenic impurity is studied in the asymmetric triple GaAs/$Al_xGa_{1-x}As$ square quantum wires. The calculations are performed using the finite difference method and a variational approach within the effective mass approximation. It is determined that the impurity binding energy strongly depends on the external electric field. The results obtained may hopefully be guiding in experiments and technological applications.

Keywords: Quantum well wire, impurity, finite difference method.

INTRODUCTION

Many studies on the energy states of an electron confined in the quantum well wires (QWWs) have been carried out because of their possible technological applications in optoelectronics [1-8]. The electronic and optical properties of electronic devices fabricated from QWWs as two-dimensional semiconductor multiple structures are strongly affected by the location of the impurity atom and the external fields such as electric, magnetic and laser fields [1-6]. Application of an electric field to a QWW causes changings in the structure's geometry and therefore a shift in its electronic levels and a redistribution of the density of states [4].

Arraoui et al. [9] studied engineering donor binding energy and polarizability in triple quantum wires. The binding energy of the donor impurity in triple graded $GaAs/(Ga,Al)As$ quantum wells was calculated by Sari et al. [10]. They obtained results in the presence of a uniform magnetic and electric field applied along the growth direction as a function of the impurity position. They showed that by changing the intensity of the external magnetic and electric field, a large spread in the range of the donor binding energy may be obtained.

In this study, it is investigated that how the application of external electric field to the asymmetric triple $GaAs/Al_xGa_{1-x}As$ square QWWs affects the impurity binding energy.

THEORY

The structural appearance of the asymmetric triple $GaAs/Al_xGa_{1-x}As$ square QWWs system examined in this study is given in Fig. 1.

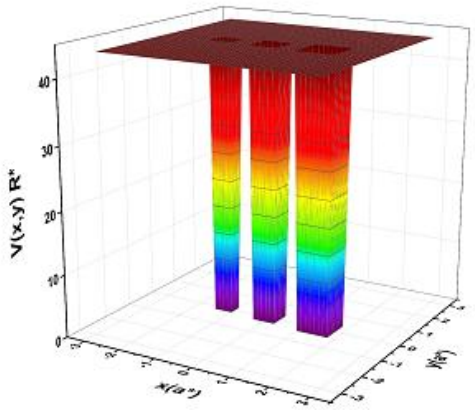


Fig.1. *A view of the considered asymmetric triple $GaAs/Al_xGa_{1-x}As$ square QWWs system*

This is an open access article licensed under Creative Commons Attribution 4.0 International
Print ISSN: 1313-230X, Online ISSN: 3033-1404

We consider that an electric field is applied to the system in the $+x$ direction. The Hamiltonian for an electron in this system under the influence of the electric field is given as follows:

$$H = \frac{\vec{p}^2}{2m^*} + |e|Fx + V(x,y) \qquad (1)$$

where effective-mass and momentum operator of the electron are denoted by m^* and $\vec{p}$, respectively. e is the elementary charge. F defines the strength of the electric field and $V(x,y)$ is the confining potential. Using the reduced units of length and energy such as a^* $(= \hbar^2\varepsilon/m^*e^2)$ and $R^*(= m^*e^4/2\hbar^2\varepsilon^2)$, respectively, and for $\vec{p} = -i\hbar\vec{\nabla}$ the Hamiltonian in Eq. 1 can be written as

$$H_1 = -\nabla^2 + \eta x + V(x,y) \quad , \qquad (2)$$

where $\eta = |e|a^*F/R^*$. First, the numerical solutions of the considered system without the impurity can be found by using the finite difference technique [4] and the following equation

$$H_1\Psi_1(x,y) = E_1\Psi_1(x,y) \quad , \qquad (3)$$

where $\Psi_1(x,y)$ and E_1 are the ground-state wave function and energy, respectively. H_1 in Eq. 3 is given by

$$H_1 = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + \eta x + V(x,y) \quad . \ (4)$$

With an impurity located at $x = x_i$, $y = 0$, and $z = 0$, the Hamiltonian equation including the Coulomb term can be written

$$H_2 = H_1 - \frac{\partial^2}{\partial z^2} - \frac{2}{\sqrt{z^2+y^2+(x-x_i)^2}}. \quad (5)$$

Then, E_{imp}, which is defined as the ground-state energy of the considered system with an impurity is obtained using the equation

$$E_{imp} = \langle\Psi_2(x,y,z)|H_2|\Psi_2(x,y,z)\rangle \, , \quad (6)$$

where the trial wave function $\Psi_2(x,y,z)$ is

$$\Psi_2(x,y,z) = N_2\Psi_1(x,y)e^{-\sqrt{z^2+y^2+(x-x_i)^2}/\lambda} \, . \qquad (7)$$

In Eq.7, N_2 is the normalization constant and λ is a variation parameter found by the minimization of E_{imp}. The impurity binding energy is given by

$$E_B = E_1 - E_{imp} \quad , \qquad (8)$$

and can be calculated as

$$E_B = -\frac{1}{\lambda^2} + \frac{2I_1}{I_2} \quad , \qquad (9)$$

where I_1 and I_2 are

$$I_1 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} K_0\left(\frac{2\sqrt{(x-x_i)^2+y^2}}{\lambda}\right) \mathrm{x}\Psi_1^2(x,y)dxdy \quad , \quad (10)$$

and

$$I_2 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \sqrt{(x-x_i)^2+y^2}K_1\left(\frac{2\sqrt{(x-x_i)^2+y^2}}{\lambda}\right) \mathrm{x}\Psi_1^2(x,y)dxdy \quad , \qquad (11)$$

where K_0 and K_1 indicate the first-order modified Bessel functions [4].

RESULTS AND DISCUSSIONS

The results are presented in the reduced effective units of length and energy, which are given by an effective Bohr radius $a^*(\cong 100\,\text{Å})$ and effective Rydberg $R^*(\cong 5.83\,meV)$, respectively. A potential barrier of $V_0 = 228\,meV$ is considered. The thicknesses of the wire on the left, at the center and on the right are taken as $0.6a^*$,$0.8a^*$ and $1a^*$, respectively, while the thicknesses of the two barriers between the three wires are taken as $0.5a^*$ in all calculations.

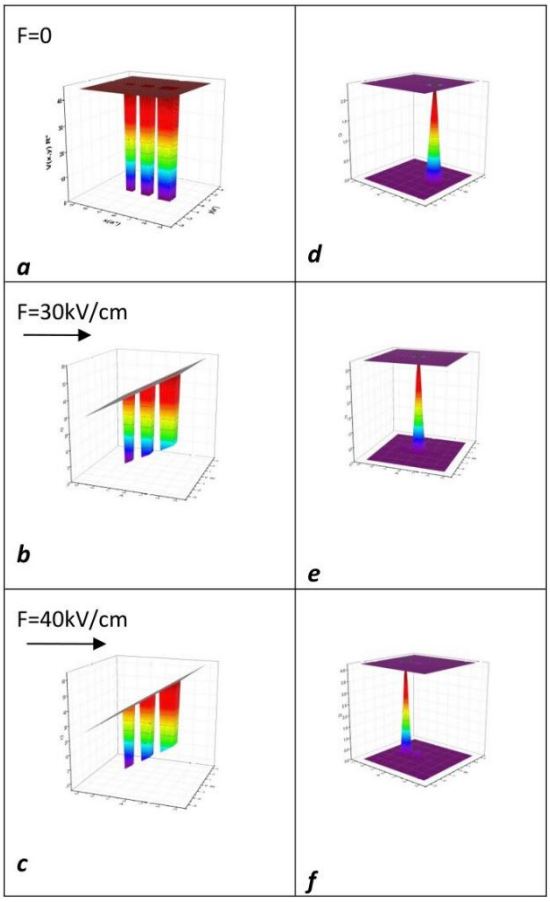


Fig. 2. *The potential profiles and the ground-state wave functions of electron for the asymmetric triple QWWs in the absence of an electric field and for the electric field intensity of F=30kV/cm and F=40kV/cm*

In the three-wire system shown in Fig. 2a—where the potential profile is depicted in the absence of an electric field—the electron is observed to be fully localized on the right-hand side wire, as seen in Fig. 2d. Fig. 2b illustrates the system's potential profile when a field of $F = 30\ kV/cm$ is applied in the $+x$ direction; in this case, the electron tunnels to the middle wire, as shown in Fig. 2e. Fig. 2c displays the potential profile for a field strength of $F = 40\ kV/cm$ (again in the $+x$ direction), where the electron transfers completely to the left-hand side wire.

To investigate the effect of an impurity atom in a quantum wire system, the dependence of the ground-state energy level E_1 (given in Eq. 8) on the electric field strength has first be calculated. It is observed from Fig. 3 that this variation increases linearly from a value of $12.5\,R^*$ at $F = 0$ to $16\,R^*$at $F = 20\ kV/cm$, remains virtually constant at $16\,R^*$ up to $F = 40\ kV/cm$, and subsequently decreases linearly at electric field strengths exceeding this value.

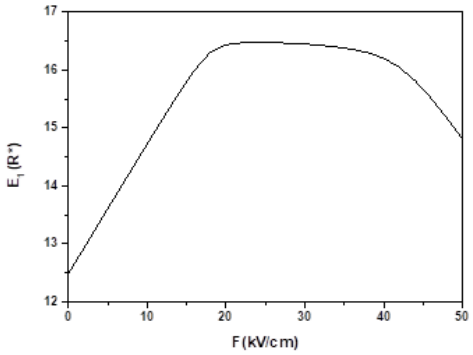


Fig. 3. *Variation of the ground-state energy of an electron in the asymmetric triple QWWs with the electric field intensity.*

The next step in investigating the impurity effect is to calculate the impurity energy level E_{imp} in Eq.8 as a function of electric field strength. Fig. 4 presents the results obtained in this regard. As can be seen, the behavior of E_{imp} closely resembles that of E_1. The function increases linearly from a value of $12\,R^*$ at $F = 0$ to an energy of $15.5\,R^*$ at $F \cong 15\ kV/cm$; it decreases with a slight slope up to $F \cong 35\ kV/cm$, and subsequently decreases exponentially at electric field strengths exceeding this value.

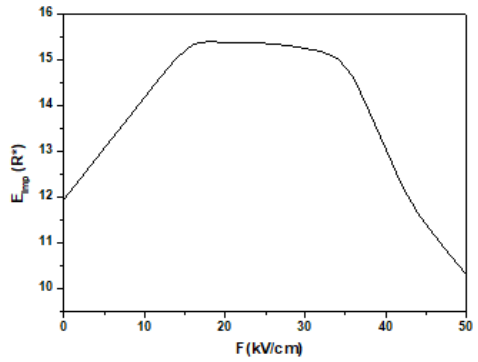


Fig. 4. *Variation of the impurity's energy in the asymmetric triple QWWs with the electric field intensity*

One can easily obtain the impurity binding energy either taking the difference E_1-E_{imp} having calculated them separately or using its expression given in Eq.9. On the assumption that an impurity atom is placed in the center of left-hand side wire, how the impurity binding energy is affected by the electric field are presented in Fig. 5.

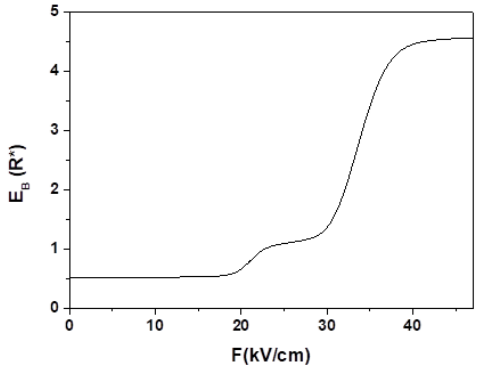


Fig. 5. *Variation of the impurity binding energy with electric field intensity for the asymmetric triple QWWs when the impurity atom is located in the center of the left wire.*

As can be seen in Fig. 5, the binding energy remains constant with increasing electric field until $F \cong 20\ kV/cm$ and then exhibits a small increase up to the to the electric field of $F \cong 30\ kV/cm$. We can explain the reason for this behavior as follows. First, the electron is located in the right-hand side wire since it is wider than the others, and the electron is far from the impurity (Fig. 2d). Because of that, the binding energy is small and constant until the electric field value reaches to $F \cong 20\ kV/cm$. Then, the electron leaks into the center wire up to and $F \cong 30\ kV/cm$. While in the center wire, the electron comes closer to the impurity with a slight increase in the binding energy. For the field strengths greater than $F \cong 30\ kV/cm$, the electron is transferred into the left-hand side wire where the impurity atom is also located (Fig. 2f), resulting in a sharp increase in the binding energy because the impurity ion and electron is now much closer in comparison with the other electron locations. After that, the binding energy is not affected from increasing electric field intensity, and keeps constant.

CONCLUSION

By using the finite difference method and a variational approach, the effect of electric field on the impurity binding energy in the asymmetric triple QWWs was investigated. The results showed that the electric field applied to the system have significant effects on the impurity binding energy. Especially it is step function-like appearance. The obtained results may hopefully guide experimenters who study QWWs.

REFERENCES

[1] Unal VU, Tomak M, Aksahin E. The effect of Coulomb interaction on optical absorption of a quantum well wire. Physica B 2024;680:415799.

[2] Pramjorn N, Amthong A. Donor binding energies in a curved two-dimensional electron system. Applied Surface Science 2020;508:145195.Bekar B, Boz FK, Aktas S, Okan SE. The Effect on the Optical Absorption Coefficients due to the Positions in the Plane of Square GaAs/Al (GaAs) Quantum Well Wire

under the Laser Field. Acta Physica Polonica A 2019;136:882.
[4] Aktas S, Boz FK, Bilekkaya A, Okan SE. The electronic properties of a coaxial square GaAs/AlxGa1-xAs quantum well wire in an electric field. Physica E. 2009;41:1572–1576.
[5] Kes H, Okan SE, Aktas S. The exitons in infinite potential centered multilayered coaxial quantum wire and the magnetic field effects on their properties. Superlattices and Microstructures 2020;139:106421.
[6] Joonhuay J, Sathongpaen P, Amthong A. Structural design of triangular core–shell nanowires for sensing polarized mid-infrared light. Materials & Design. 2023;230:111983.
[7] Hu M, Wang H, Gong Q. The impurity states in InGaAsP/InP coaxial double quantum well wires with the effects of electric and magnetic fields. Modern Physics Letters B. 2021;35:2150355.
[8] Bilekkaya A, Aktas S, Okan SE, Boz FK. Electric and magnetic field effects on the binding energy of a hydrogenic impurity in quantum well wires with different shapes. Superlattices and Microstructures 2008;44:96–105.
[9] Arraoui R, Jaouanne M, Ben Hammou O, El-Hamouchi J, Ed-Dahmouny A, Fakkahi A, Sali A. Engineering donor binding energy and polarizabilty in triple quantum wire nanosystems. Materials Science and Engineering B 2026;332:119602.
[10] Sari H, Kasapoglu E, Sokmen I. Shallow donors in a triple graded quantum well under electric and magnetic field. Physica B 2003;325:300.