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ARISTON PUBLICATIONS
Quantum Advances
ISSN: 3143-0724 www.aristonpubs.com/journal/quantum-advances https://doi.org/10.69626/qa.2026.0097

RESEARCH ARTICLE

Electronic properties of the asymmetric double GaAs/AlxGa$_{1-x}$As quantum wires

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ABSTRACT: The electronic properties of asymmetric double GaAs/Al$_x$Ga$_{1-x}$As cylindrical quantum wires are theoretically investigated, with particular emphasis on the binding energy of a hydrogenic impurity under the combined influence of external electric and magnetic fields. Using the effective mass approximation, the single-particle Schrödinger equation is solved through a hybrid approach combining the finite difference method for the electron ground state and a variational technique for the impurity problem. The confining potential consists of two cylindrical quantum wires of different radii separated by a thin barrier, creating an asymmetric structure that allows for unique tuning of electronic states. The calculations examine various impurity positions within the structure, specifically considering impurities located at the center of either the left or right wire, while systematically varying the electric field strength up to 45 kV/cm and magnetic field intensities up to 1.5 T. The results reveal that the impurity binding energy exhibits pronounced sensitivity to all investigated parameters, displaying sharp transitions between distinct binding energy regimes as external fields modify the confinement potential. When the impurity resides in the smaller left wire, increasing electric fields cause the binding energy to undergo an abrupt step-like enhancement, attributed to field-induced transfer of the electron wavefunction from the larger to the smaller wire. Conversely, impurities positioned in the larger right wire experience a sudden decrease in binding energy under similar conditions. The magnetic field is found to shift these transition thresholds toward lower electric field values, facilitating the electron transfer process through enhanced spatial confinement. These findings provide valuable insights for the design of tunable quantum devices and may serve as a practical guide for experimental investigations of low-dimensional semiconductor structures, particularly in applications requiring controlled manipulation of impurity states through external fields.

Keywords: Quantum Well Wire, Impurity, Finite Difference, Binding Energy, Electric Field, Magnetic Field.

Received: 08 July 2026; Revised: 13 August 2026; Accepted: 02 September 2026; Published Online: 12 September 2026

1. INTRODUCTION

The relentless pursuit of miniaturization in electronic and optoelectronic devices has driven intensive research into low-dimensional semiconductor structures over the past several decades. Quantum wells (QWs), quantum well wires (QWWs), and quantum dots (QDs) represent successive stages of quantum confinement, where charge carriers are restricted in one, two, or three spatial dimensions, respectively. This dimensional confinement gives rise to discrete energy levels and modified density of states, fundamentally altering the electronic and optical properties of materials compared to their bulk counterparts. Among these structures, QWWs—also referred to as quantum wires or nanowires—occupy a particularly important position as they combine the advantages of onedimensional transport with enhanced quantum confinement effects, making them promising candidates for high-performance transistors, laser diodes, photodetectors, and quantum information processing applications [1–18].

The electronic and optical properties of devices fabricated from QWWs are profoundly influenced

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by several factors, including the presence of impurity atoms and the application of external fields such as electric, magnetic, and laser fields [1–7]. Impurities, whether intentionally introduced through doping or present as residual contaminants, play a dual role in semiconductor devices: they can serve as donors or acceptors that modulate carrier concentrations, or they can act as scattering centers that degrade device performance. Understanding the binding energy of hydrogenic impurities in QWWs is therefore of fundamental importance, as this parameter directly affects carrier mobility, optical transition energies, and the overall device response. Hydrogenic impurities, which consist of a charged impurity center binding an electron (or hole) through Coulomb interaction, provide an ideal model system for studying impurity-related phenomena in confined geometries. The binding energy of such impurities is highly sensitive to the degree of quantum confinement, the impurity position relative to the structure boundaries, and any external perturbations applied to the system. The application of electric and magnetic fields to QWW structures introduces additional degrees of freedom for controlling electronic properties. An external electric field modifies the confinement potential by tilting the band profile, thereby shifting electronic levels and altering the spatial distribution of the wavefunction [2–10]. This field-induced redistribution of the wavefunction can significantly affect the overlap integral between the electron and its parent impurity center, leading to dramatic changes in the impurity binding energy. Similarly, a magnetic field applied perpendicular to the wire axis introduces additional confinement through the Lorentz force, compressing the electron wavefunction and modifying the effective dimensionality of the system. The combined action of electric and magnetic fields creates a rich and complex landscape of possible electronic configurations, offering unprecedented opportunities for tuning device characteristics through external control parameters. Numerous theoretical investigations have explored impurity states in various QWW geometries. Chouef et al. [11] systematically examined the effects of surface curvature and electric field on the electronic and optical properties of off-center hydrogenic donor impurities in two-dimensional nanostructures, highlighting the importance of geometric factors in determining impurity behavior. Tangarife and Duque [12] calculated impurity binding energies in symmetric double QWWs under an electric field, revealing that the binding energy can either increase or decrease depending on the direction of the applied field and the impurity position within the structure. This directional dependence arises from the asymmetric perturbation of the confinement potential, which can either enhance or suppress the electron-impurity Coulomb interaction. Hu et al. [13] investigated impurity states in InGaAsP/InP coaxial double QWWs under combined electric and magnetic fields, demonstrating that both fields exert significant influence on the binding energy for different impurity positions. Restrepo et al. [14] studied double QWWs with a W-shaped potential profile under electric field and hydrostatic pressure, showing that these external factors, along with the potential barrier shape, strongly affect the impurity binding energy. The impurity binding energy in asymmetric and symmetric binary GaAs/AlGaAs square quantum wires under electric and magnetic fields was reported by Bilekkaya [15], who found pronounced field-dependent effects. Kasapoglu and Duque [16] calculated the electronic structure and optical absorption coefficient of Manning-like double quantum wells under external fields, establishing that the electronic properties can be systematically adjusted by varying structural parameters such as well and barrier widths, well depth, and inter-well coupling, in addition to external field intensities. More recently, Aydin and Sahin [17] performed a detailed investigation of the electronic properties of two-electron core/shell/well/shell quantum dot heterostructures, systematically comparing cases with and without on-center donor impurities. Unal et al. [1] examined the effect of Coulomb interaction on optical absorption in quantum well wires, while Pramjorn and Amthong [2] calculated donor binding energies in curved two-dimensional electron systems. Despite the extensive body of work on impurity states in QWWs, the specific case of asymmetric double cylindrical QWWs under combined electric and magnetic fields remains relatively unexplored. Asymmetric double QWW structures, where the two constituent wires have different radii or confining potentials, offer unique possibilities for controlling electronic states through external fields. The asymmetry introduces additional tunability, as the different confinement strengths in the two wires create distinct energy levels that can be selectively shifted by applied fields, potentially leading to field-induced electron transfer between the wires. Such structures could serve as the basis for novel switching or sensing devices where the impurity binding energy acts as a sensitive probe of external conditions. The aim of this study is to systematically investigate the effect of external electric and magnetic fields on the impurity binding energy in asymmetric double GaAs/Al$_x$Ga$_{1-x}$As cylindrical QWWs. In addition, the influence of impurity location on the binding energy is thoroughly examined. For this purpose,

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the single-particle Schrödinger equation is solved within the effective-mass approximation, employing a combination of the finite difference method for numerical solution of the field-free Hamiltonian and a variational approach for the impurity problem. The remainder of this paper is organized as follows: Section 2 presents the theoretical framework and the mathematical formulation of the problem, including the Hamiltonian, confinement potential, and the variational procedure. Section 3 discusses the numerical results, examining the effects of electric field, magnetic field, and impurity position on the binding energy. Finally, Section 4 summarizes the main findings and provides concluding remarks.

2. THEORY

The structural form of the asymmetric double GaAs/AlxGa1-xAs cylindrical QWWs system examined in this study is given in Figure 1.

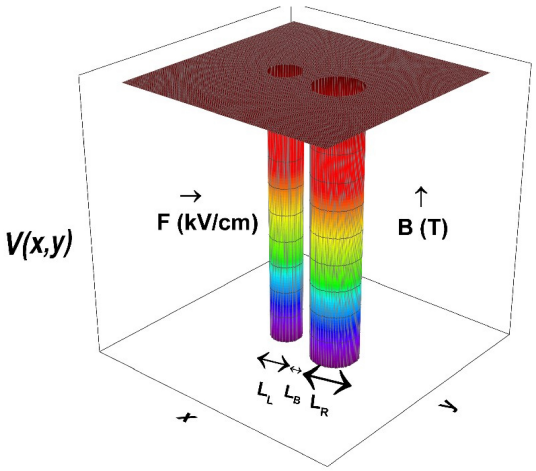


Fig. 1. The structural form of the considered asymmetric double GaAs/AlxGa$_{1-x}$As cylindrical QWWs system.

Using the effective-mass approximation, the Hamiltonian equation of the studied double QWWs system lying along the +z direction, under an electric field applied in the +x direction and uniform magnetic field in the +z direction is taken to be

$$H_0 = \frac{1}{2m^*}\left[\vec{p} + \frac{e\vec{A}}{c}\right]^2 + |e|Fx + V(x,y) \tag{1}$$

where the effective mass and momentum operator of the electron are denoted by m^* and $\vec{p}$, respectively. e is the elementary charge. The potential $\vec{A}$ is chosen as

$$\vec{A} = \left(-\frac{1}{2}By, \frac{1}{2}Bx, 0\right),$$

yielding

$$\vec{B} = (0, 0, B).$$

F defines the strength of the electric field and $V(x,y)$ is the confining potential. The mathematical expression of the confinement potential is given by

$$V(x,y) = \begin{cases} 0, & -\frac{L_L}{2} \le y \le \frac{L_L}{2}, \\ & -\frac{L_B}{2} - L_L \le x \le -\frac{L_B}{2}, \\ 0, & -\frac{L_R}{2} \le y \le \frac{L_R}{2}, \\ & \frac{L_B}{2} \le x \le \frac{L_B}{2} + L_R, \\ V_0, & \text{otherwise.} \end{cases} \tag{2}$$

where L_L is the diameter of the left cylindrical wire, L_B is the thickness of the barrier between the two wires, and L_R is the diameter of the right cylindrical wire.

By using

$$\vec{p} = -i\hbar\vec{\nabla},$$

and reduced units a^* for length and R^* for energy units, the Hamiltonian in Eq. (1) can be rewritten as

$$H_0 = -\nabla^2 + \eta x + \gamma L_z + \frac{\gamma^2}{4}(x^2 + y^2) + V(x,y) \tag{3}$$

where

$$\gamma = \frac{e\hbar B}{2m^* c R^*}$$

and

$$\eta = \frac{|e|a^* F}{R^*}$$

are zero-dimensionless measurements of the magnetic and electric fields, respectively. B is the applied magnetic field strength, and L_z indicates the z component of the angular momentum operator.

By employing the finite difference technique, the exact numerical solutions of the studied QWWs can be obtained from the following equation:

$$H_1\Psi_1(x,y) = E_1\Psi_1(x,y) \tag{4}$$

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where E_1 and $\Psi_1(x,y)$ are the ground-state energy and corresponding wave function, respectively. H_1 in Eq. (4) is given by

$$H_1 = -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} + \eta x + \frac{\gamma^2}{4}(x^2+y^2) + V(x,y) \tag{5}$$

The finite difference method is employed to obtain the numerical solutions to Eq. (1). The details of the numerical calculations are given elsewhere [**? ?**]. With an impurity located at $x = x_i$, $y = 0$, and $z = 0$, the Hamiltonian equation including the Coulomb term can be written as

$$H_2 = H_1 - \frac{\partial^2}{\partial z^2} - \frac{2}{\sqrt{z^2+y^2+(x-x_i)^2}} \tag{6}$$

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

$$E_{\text{imp}} = \langle \Psi_2(x,y,z)|H_2|\Psi_2(x,y,z)\rangle \tag{7}$$

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

$$\Psi_2(x,y,z) = N_2\Psi_1(x,y) \times \exp\left[-\frac{\sqrt{z^2+y^2+(x-x_i)^2}}{\lambda}\right] \tag{8}$$

In Eq. (8), N_2 is the normalization constant, and λ is a variational parameter determined by minimizing E_2. The impurity binding energy is given by

$$E_B = E_1 - E_{\text{imp}} \tag{9}$$

and can be calculated as

$$E_B = -\frac{1}{\lambda^2} + \frac{2I_1}{I_2} \tag{10}$$

where I_1 and I_2 are

$$I_1 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} K_0\left(\frac{2\sqrt{(x-x_i)^2+y^2}}{\lambda}\right) \times \Psi_1^2(x,y)\,dx\,dy \tag{11}$$

and

$$I_2 = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \sqrt{(x-x_i)^2+y^2} \times K_1\left(\frac{2\sqrt{(x-x_i)^2+y^2}}{\lambda}\right)\Psi_1^2(x,y)\,dx\,dy \tag{12}$$

where K_0 and K_1 indicate the first-order modified Bessel functions [5, 15].

3. RESULTS AND DISCUSSION

The results are presented in reduced effective units of length and energy, given by the effective Bohr radius a^* and effective Rydberg energy R^*, respectively. The values of them are $a^* \cong 100$ Å and $R^* \cong 5.83\ meV$ in GaAs/Al$_x$Ga$_{1-x}$As QWWs. The static dielectric constant of $GaAs$, $\varepsilon = 12.5$ is considered equivalent in all structure. The effective mass of the hydrogenic donor is assumed as $m^* = 0.067m_0$ where m_0 is the free-electron mass and the Al concentration x is taken as 0.3 which forms the potential energy of $V_0 \cong 228\ meV \cong 39,1R^*$. In this study, and values

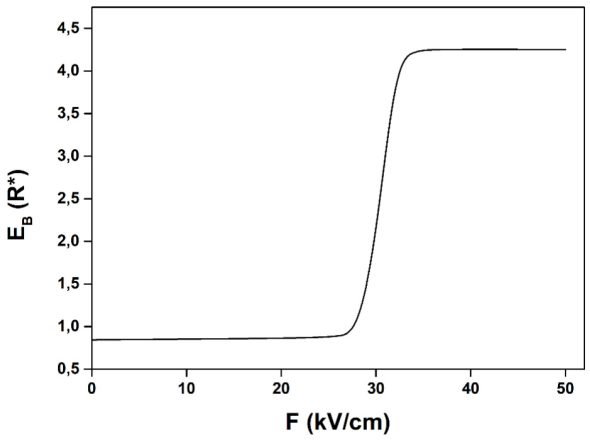


Fig. 2. The impurity binding energy as a function of the electric field for the asymmetric QWWs when the impurity atom is located in the center of the left wire.

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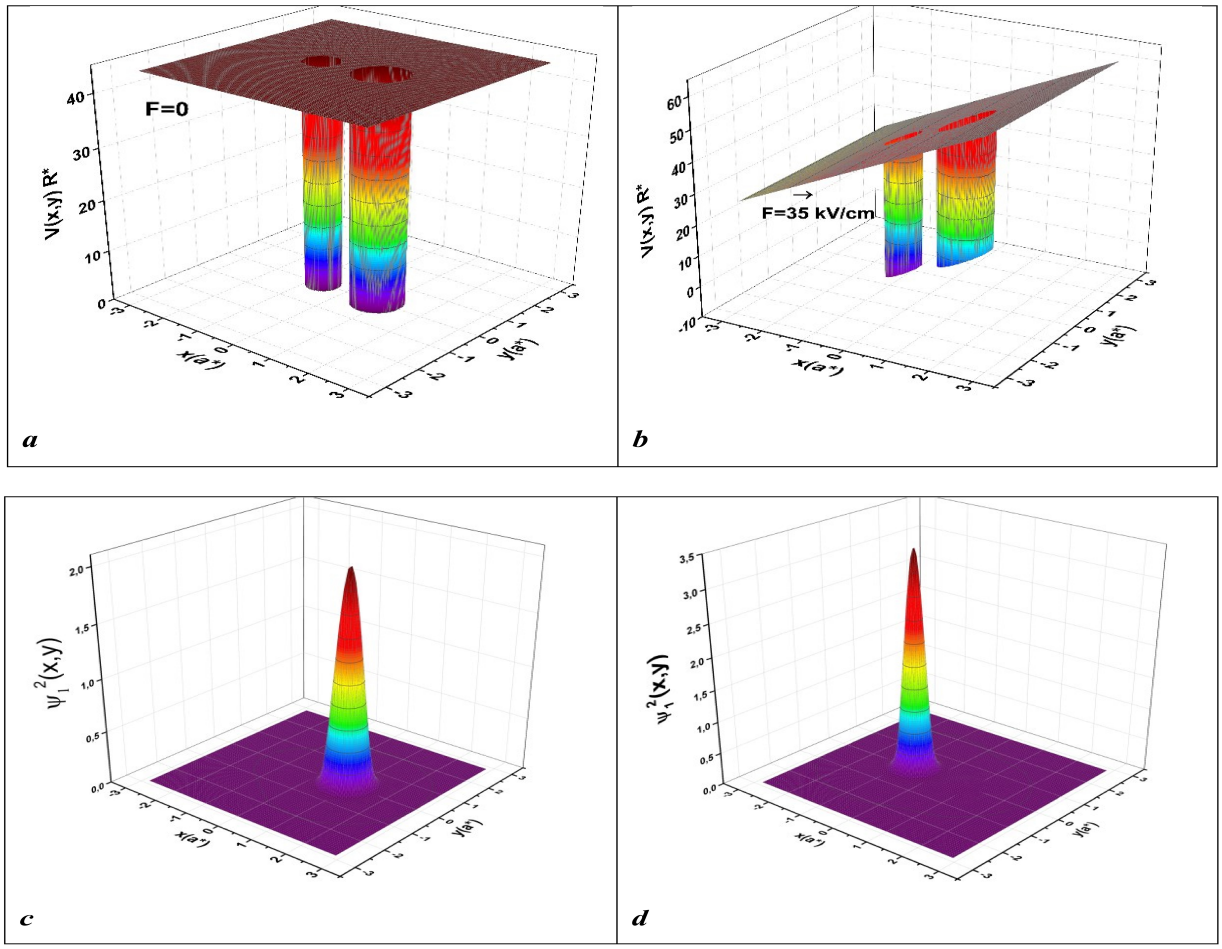


Fig. 3. Potential profiles and electron's probability distributions for the asymmetric QWWs for F=0 and F=35 kV/cm applied in direction, respectively.

are kept constant as $LL = 0.8a^*$, $LB = 0.5a^*$, and $LR = 1.2a^*$ in all calculations. We first examined how the impurity binding energy is affected by the electric field which is applied in the direction assuming that the impurity atom is in the center of the left wire. Figure 2 depicts the binding energy changes of the impurity as a function of the magnitude of the electric field strength.

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As shown in the figure, the coupling energy remains almost constant up to an electric field strength of approximately 28 kV/cm, then increases almost sharply (like a smooth step function), and becomes constant again after an electric field strength of approximately 33 kV/cm. The underlying reason for this sharp increase in the binding energy in the asymmetric QWWs exhibited in Figure 2 can be explained by viewing the potential profiles and the wave functions of electron as shown in Figure 3. The potential profiles of the system and the ground-state probability distributions of electron in the asymmetric QWWs in the absence of an electric field ($F = 0$) and for the electric field of $F = 35$kV/cm applied in the direction are shown in Figure 3. Figure 3a and 3c present the potential profile of the asymmetric QWWs for and the corresponding electron's probability distribution

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for that profile, respectively, while Figure 3b and 3d are the potential profile for $F = 35$kV/cm and corresponding probability distribution, respectively. When there is no electric field, the electron is confined almost entirely to the right wire, as shown in Figure 3c, because it has a larger volume. Due to the attractive Coulomb interaction of the donor ion, the electron wave function can penetrate somewhat into the left region, but this is not so drastic. When the external electric field is applied in the x-direction, the potential profile of the structures is perturbed, and the depth of the left wire increases while that of the right wire decreases, as seen in Figure 3b. Therefore, in addition to the attractive property of the donor ion, this increasing depth causes more penetration of the electron into the left region due to the minimum energy principle and results in higher binding energy. When the external electric field strength reaches a certain value, such as 35kV/cm, the electron is completely confined to the left wire, as seen in Figure 3d. That is, the electron and impurity atom are in the same spatial region, and the binding energy reaches the highest value. After that stage, the binding energy is unaffected by further increases in the electric field and remains constant.

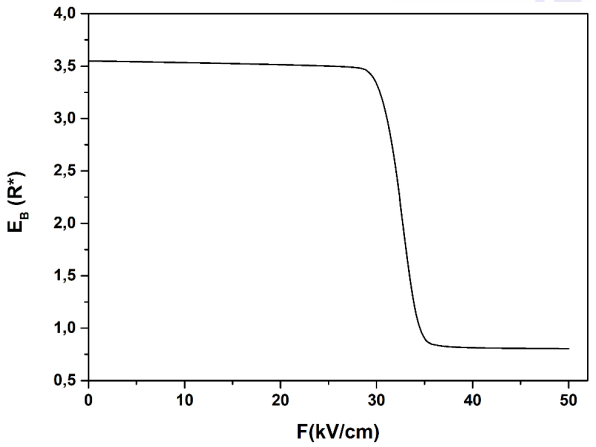


Fig. 4. The impurity binding energy as a function of the electric field for the asymmetric QWWs when the impurity atom is located in the center of the right wire.

Figure 4 demonstrates the impurity binding energy as a function of electric field in the asymmetric QWWs when an impurity atom is located in the center of the right confinement region, as different from Figure 2. It is noted that the electric field direction is the same as that of Figure 2. It is observed that the binding energy remains approximately constant at $3.5R^*$ as the electric field strength increases, then drops rapidly to $0.75R^*$ between $F = 29 - 36$ kV/cm (like an inverse step function), and the binding energy value becomes approximately constant at this value with further increases in the electric field strength. This is because an increase in the electric field results in a deeper potential profile in the left confinement region and a shallower potential profile in the right confinement region. When the electric field strength is 36 kV/cm, the resulting perturbation in the confinement potentials suppresses the attractive Coulomb potential of the donor ion, and the electron is confined almost completely in the left well, although its smaller volume. Finally, in the asymmetric QWWs, the variation in binding energy in the presence of an external magnetic field is investigated as a function of the electric field. The results are shown in Figure 5.

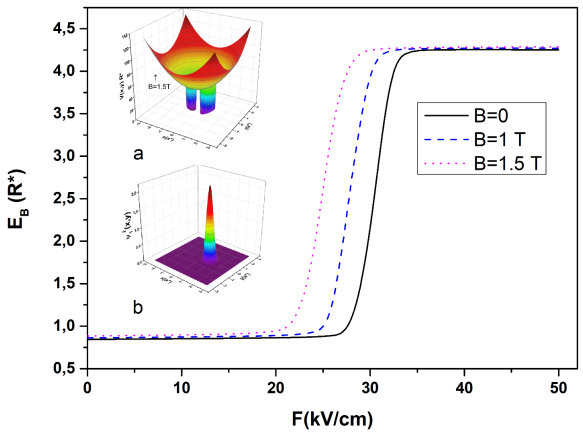


Fig. 5. The impurity binding energy as a function of the electric and magnetic fields simultaneously applied to the symmetric QWWs when the impurity atom is located in the center of the left wire. Insets (a) confinement potential shape when B=1.5 T and (b) electron's probability distribution when B=1.5 T

The insets (a) and (b) show the potential profile and the ground-state probability distribution of electron for $B = 1.5$ T, respectively. The calculations were performed assuming that the impurity atom was in the left wire and that the magnetic field is applied in the $+z$ direction while the electric field's direction is $+x$. As seen in Figure 5, the behavior of the binding energy with increasing electric field strength and its transition between minimum and maximum values are the same as in Figure 2. But the transition region is firmly dependent on the magnetic field strength. The transition from a lower to a higher binding energy occurs at lower electric field strengths as the external magnetic field strength increases. While that transition is around $F = 30$ kV/cm in the absence of a magnetic field, it shifts to smaller electric field values as the magnetic field is increased. For example, the sharp transition occurs around $F = 25$ kV/cm for $B = 1.5$ T. With the magnetic field, the electron is transferred more easily from the right wire to the left wire, where the impurity atom is located at smaller electric field values, and thus sharp increases in the binding energy are observed.

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4. CONCLUSION

In this study, the electronic properties of asymmetric double GaAs/Al$_x$Ga$_{1-x}$As cylindrical quantum well wires have been systematically investigated using the finite difference method combined with a variational approach within the effective-mass approximation. The primary focus was on understanding how the binding energy of a hydrogenic impurity is influenced by external electric and magnetic fields, as well as by the impurity position within the asymmetric structure. The results demonstrate that the impurity binding energy exhibits remarkable sensitivity to all applied external perturbations. Specifically, when the impurity is located in the smaller left wire, increasing the electric field strength leads to an abrupt step-like enhancement of the binding energy, attributed to fieldinduced electron transfer from the larger right wire to the left wire where the impurity resides. Conversely, when the impurity is positioned in the larger right wire, the binding energy undergoes a sudden drop under similar field conditions, as the electron becomes confined to the opposite wire. The application of a magnetic field shifts these sharp transition thresholds toward lower electric field values, facilitating electron transfer through enhanced spatial confinement. These findings highlight the possibility of actively controlling impurity states in asymmetric double QWW structures by appropriately tuning external field parameters. The results presented herein may serve as a valuable reference for experimental investigations of QWW-based devices and could potentially guide the design of novel quantum structures where impurity binding energy can be modulated for specific technological applications, such as tunable detectors, switches, or sensors operating in the lowdimensional regime.

DECLARATIONS

Ethical Approval

We affirm that this manuscript is an original work, has not been previously published, and is not currently under consideration for publication in any other journal or conference proceedings. All authors have reviewed and approved the manuscript, and the order of authorship has been mutually agreed upon.

Funding

Funding not available

Availability of data and material

The datasets used and/or analyzed during the current study are available from the corresponding author on reasonable request.

Authors' contributions

All the authors contributed substantially to the paper.

Conflicts of Interest

The authors declare that they have no financial or personal interests that could have influenced the research and findings presented in this paper. The authors alone are responsible for the content and writing of this article.

Data Availability

This manuscript has no associated data added to any data repository.

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