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**Research Article / Araştırma Makalesi**

# THE BINDING ENERGY OF A HYDROGENIC IMPURITY IN TRIPLE GaAs/AlxGa1-xAs QUANTUM WELL-WIRES UNDER APPLIED ELECTRIC FIELD

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**Abstract:** The ground state binding energy of hydrogenic impurity in a triple GaAs/$Al_xGa_{1-x}As$ quantum well-wire (QWW) system subjected to an external electric field applied perpendicular to the along axis of the wire system is studied. The valance subband energies and wave functions in the presence of an electric field are calculated using the fourth-order Runge-Kutta method. The variational method for the binding energy of hydrogenic impurity in a triple GaAs/$Al_xGa_{1-x}As$ QWW has been used. Binding energy calculations were performed as function of the wire thickness, the electric field and the impurity position. Numerical results for binding energy of hydrogenic impurity in a triple GaAs/$Al_xGa_{1-x}As$ QWW show a sharp decrease or increase, which may be important in device applications, under suitable conditions.

***Key words:*** binding energy, electric field, triple GaAs/$Al_xGa_{1-x}As$, quantum well-wires

**Elektrik alan altında üçlü GaAs/AlxGa1-xAs kuantum kuyu-tellerinde bir hidrojenik yabancı atomun bağlanma enerjisi**

**Özet:** Tel sisteminin ekseni boyunca dik uygulanan bir dış elektrik alan etkisine maruz kalan üçlü GaAs/$Al_xGa_{1-x}As$ kuantum kuyu tel sisteminde, hidrojenik yabancı atomun taban durum bağlanma enerjisi çalışıldı. Elektrik alan etkisinde, valans subband enerjileri ve dalga fonksiyonları dördüncü derece Runge-Kutta metodu kullanılarak hesaplandı. Üçlü GaAs/$Al_xGa_{1-x}As$ kuantum kuyu telinde hidrojenik yabancı atomun bağlanma enerjisi için varyasyonel metot kullanılmıştır. Bağlanma enerjisi hesapları tel kalınlığının, elektrik alanın ve yabancı atomun konumunun fonksiyonu olarak incelenmiştir. Üçlü GaAs/$Al_xGa_{1-x}As$ kuantum kuyu telinde hidrojenik yabancı atomun bağlanma enerjisi için nümerik sonuçlar keskin bir artma veya azalma gösterir ki bu uygun şartlar mevcut olduğunda devre elemanları uygulamalarında önemli olabilir.

***Anahtar Kelimeler:*** bağlanma enerjisi, elektrik alan, üçlü GaAs/$Al_xGa_{1-x}As$ kuantum kuyu telleri.

## Giriş

Sakaki (1980) was the first to suggest mobility enhancement in thin semi-conducting wires. The electric and optical properties of semi-conducting QWWs have recently attracted considerable attention (Chao and Thoai, 1995; Ulaş et al., 1997; Thoai, 1992). Lee and Spector (1983) have first treated a hydrogenic impurity placed on the axis of QWW, assuming infinite confining potential, neglecting in this way the tunnelling effects across the surface of QWW. They have shown that the enhancement of the binding energy for the ground state is even greater than that in two dimensional quantum wells. The binding energy approaches infinity as the radius of the QWW decreases. Later on, many authors have investigated the binding energies for hydrogenic impurity states in QWWs (Vasilopoulos and Raichev, 2000; Montes et al.,1998).

The interest in these systems resides essentially in the possibility of various device applications. The effect of an applied electric field on the physical properties of such devices constitutes considerable interest. For instance, the application of an electric field in the crystal growth direction causes a polarization of the carrier distribution and shifts the quantum energy states, which can be used to control and modulate the intensity output

of the device (Aktaş et al, 2001; Chuu et al, 1992; Lee and Kim, 1998; Aghasyan and Kirakosyan, 2000, Aktaş et al., 2000). Therefore, QWWs may be very useful for the fabrication of new kinds of optoelectronic devices (Korepov and Liberman, 1999; Kim and Lee, 2000; Okan et al., 2000).

The aim of this paper is to calculate the ground state binding energy of a hydrogenic impurity in rectangular triple GaAs/$Al_xGa_{1-x}As$ QWWs depending on the electric field strength, the wire thickness and the impurity position. The geometric structure of the rectangular triple GaAs/$Al_xGa_{1-x}As$ QWW is shown schematically in figure 1.

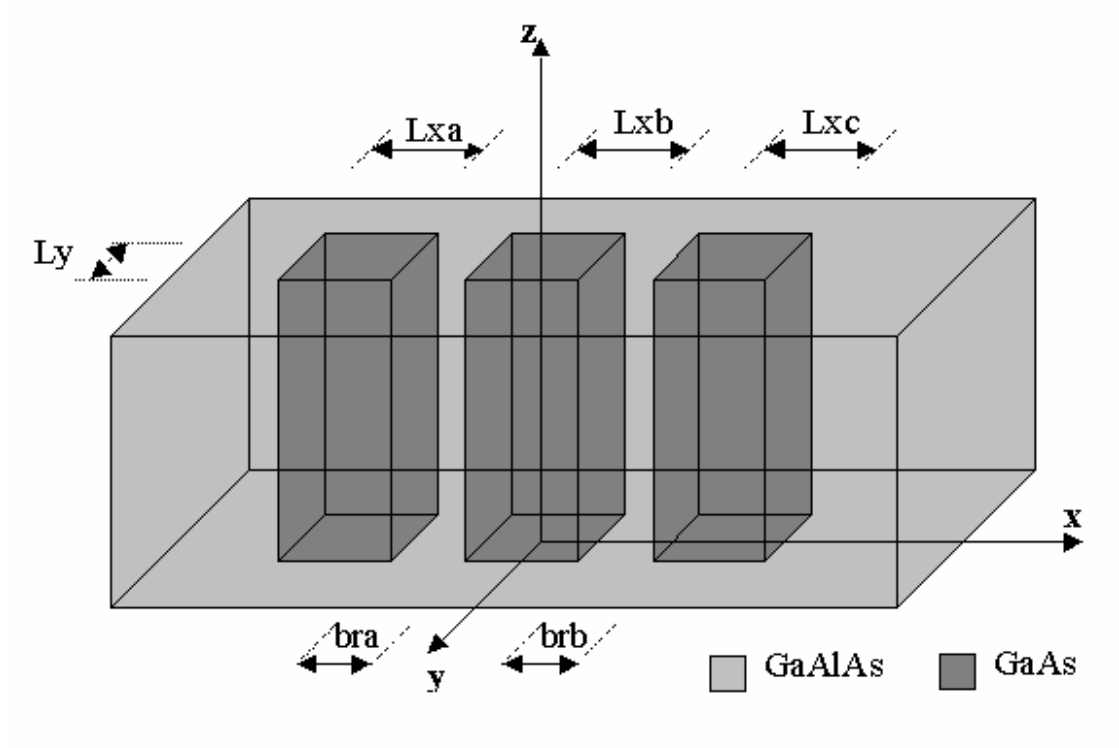


**Figure 1.** Schematic view of a rectangular triple GaAs/$Al_xGa_{1-x}As$ QWW system.

***Theory***

Let us consider a rectangular QWW placed of external electric field perpendicular to wire axis. Within the framework of the effective mass approximation, the Hamiltonian for the wire of rectangular cross-section, lying along the z-direction is given as

$$H_o = -\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+V(x,y)+eF(x\cos\theta+y\sin\theta) \qquad (1)$$

where $m^*$ is the effective mass of the electron, F is the electric field strength applied in along the $x-y$ plane and $\theta$ is the angle between the electric field and the $x$-axis. In eq. (1), the finite barrier potential $V(x,y)$ can be taken as

$$V(x,y)=\begin{cases} 0 & -\frac{Lxb}{2}-bra-Lxa\le x\le -\frac{Lxb}{2}-bra, \quad |y|<\frac{Ly}{2} \\ 0 & -\frac{Lxb}{2}\le x\le \frac{Lxb}{2}, \quad |y|<\frac{Ly}{2} \\ 0 & \frac{Lxb}{2}+brb\le x\le \frac{Lxb}{2}+brb+Lxc, \quad |y|<\frac{Ly}{2} \\ V_0 & elsewhere, \quad |y|<\frac{Ly}{2} \end{cases} \tag{2}$$

where, the electron is free to move along the z-direction but constrained along $x-$ and $y-$ directions. The ground state wave function $\psi_0(x,y)$ and the ground state energy $E_0$ are numerically obtained by using the fourth order Runge-Kutta method (Bloss, 1989). In numerical calculates it is used FORTRAN program language.

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

$$H_1 = H_0 - \frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2} - \frac{e^2}{\varepsilon\sqrt{(x-x_i)^2+(y-y_i)^2+z^2}} \tag{3}$$

where $\varepsilon$ is the static dielectric constant of the medium in which the electron moves, $\left[(x-x_i)^2+(y-y_i)^2+z^2\right]^{1/2}$ is the distance between the carrier and the impurity site. As a trial wave function for the ground state of the impurity we have used

$$\psi_1(x,y,z) = N_1\psi_0(x,y)\exp(-\sqrt{(x-x_i)^2+(y-y_i)^2+z^2}\,/\lambda) \tag{4}$$

where $N_1$ is normalization constant and $\lambda$ is the variational parameter that is determined by minimizing the expectation value $E_1$ of the Hamiltonian in eq. (3).

$$E_1 = \left[\frac{\langle\psi_1|H_1|\psi_1\rangle}{\langle\psi_1|\psi_1\rangle}\right]_{\lambda_{\min}} \tag{5}$$

The impurity binding energy $E_b$ is defined as the difference between the lowest value of the electron energy $E_0$ and the impurity energy $E_1$ (Aktaş vd. 2001, Aktaş vd. 2000).

$$E_b = E_0 - E_1 = -\frac{1}{\lambda^2}+\frac{2A}{B} \tag{6}$$

where

$$A = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dxdy\,\psi_0^2(x,y)K_0(2\sqrt{(x-x_i)^2+(y-y_i)^2}\,/\lambda) \tag{7}$$

and

$$B = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} dxdy\,\psi_0^2(x,y)\sqrt{(x-x_i)^2+(y-y_i)^2}\,K_1(2\sqrt{(x-x_i)^2+(y-y_i)^2}\,/\lambda) \tag{8}.$$

$K_0$ and $K_1$ are the zero and first- order modified Bessel functions of the second kind, respectively.

**Results and Conclusions**

In this section we carry out the numerical calculations for different cases of the triple GaAs/$Al_xGa_{1-x}As$ QWWs. The results are presented in reduced effective units of length and energy, which are given in term of effective Bohr radius $a^* = \hbar^2 \varepsilon / m^* e^2$ and effective Rydberg constant $R^* = m^* e^4 / 2\hbar^2 \varepsilon^2$ , respectively. These units are $a^* \cong 98$ Å and $R^* \cong 5.83$ meV for hydrogenic donors in GaAs/$Al_xGa_{1-x}As$ QWWs. We have considered the Al concentration $x = 0.3$ which corresponds to a potential barrier of approximately $V_o$=220 meV. The external electric field is applied in the x-direction ($\theta = 0$).

In Figs. 2 and 3, the binding energy with and without electric field are shown as a function of the outer QWWs thickness Lxa, Lxc for a hydrogenic impurity localized at the center of the inner and of the right outer QWW, respectively. In both figures, the Lxb=0.8 a* and the brb=bra=0.3 a* are constant. The Lxa=Lxc changes from 0.4 a* to 1.5a*.

In Fig. 2, the impurity is at the center of right outer wire. As Lxa=Lxc increase, a slight decrease in the binding energy is seen due to the weakening Coulomb interaction between impurity and electron for F=0. While the thickness of outer wires is small in the first, the existence probability of the electron in outer wires is also small. This causes the weakening Coulomb interaction. Therefore, the binding energy has been small. At a critical value of Lxa=Lxc($\approx 0.8$a*), the outer QWW thicknesses are bigger than the inner QWW thickness. The electron, within the inner QWW in the first place, passes to the outer QWWs with tunnelling. For this reason, the electron becomes close to the impurity. This case causes an approximately three-fold increase in the binding energy. When the electric fields, F=-5 kV/cm and F=-10 kV/cm, are applied, the binding energy shows a slight increase in comparison with the field-off case. Owing to the existence probability of electron in right outer QWW have more increased with the electric field effect, the critical transition point changes from 0.8 a* to 0.6a*.

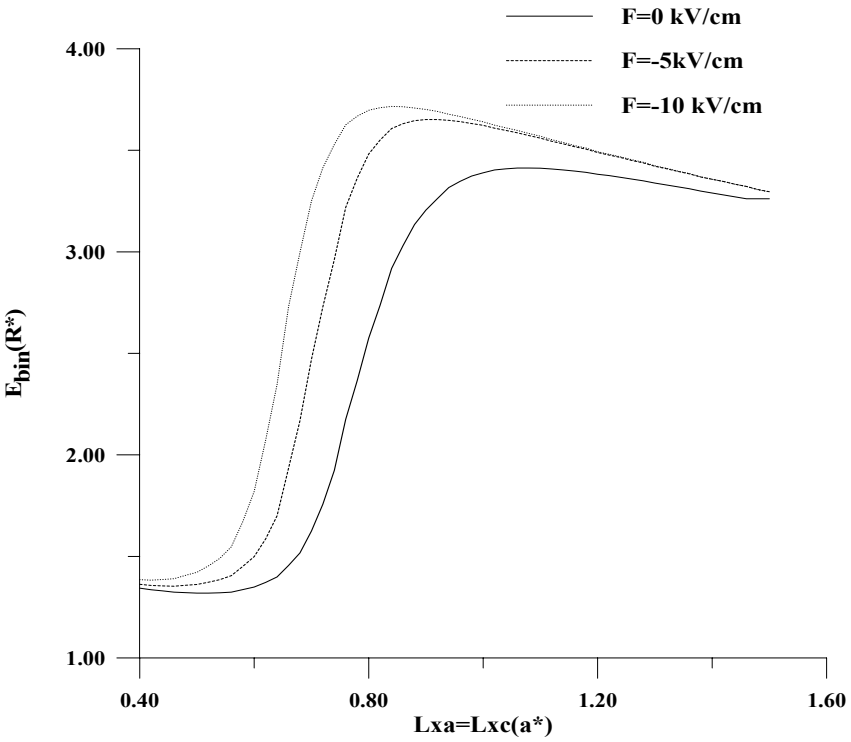


**Figure 2.** Binding energies of an electron bound to a hydrogenic impurity at the centre of right outer QWW as a function of the outer QWWs thickness Lxa=Lxc for various electric field strengths.

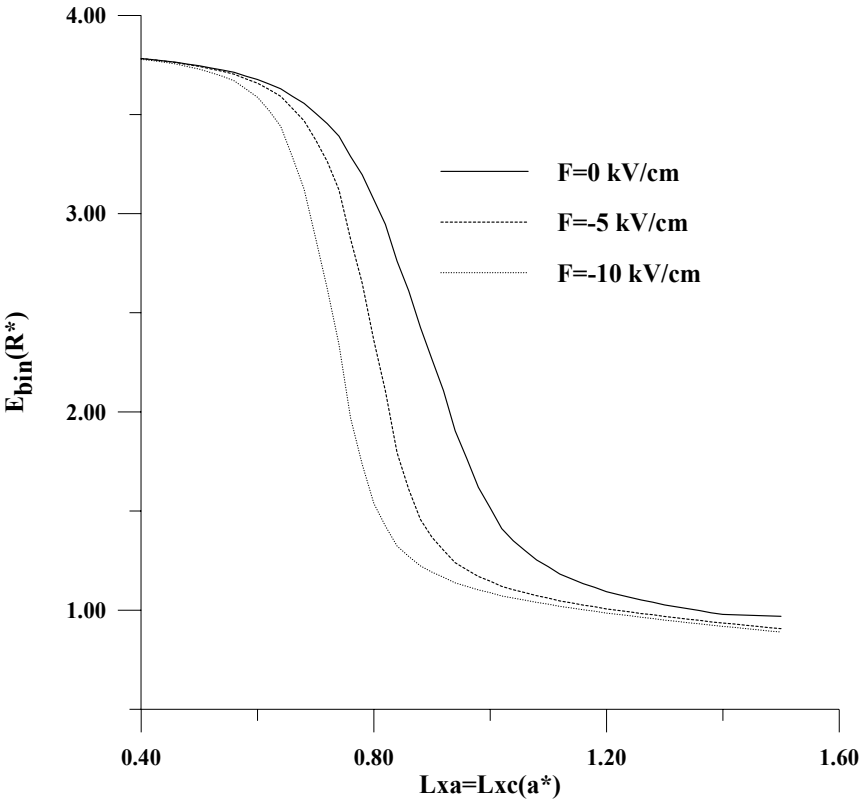


**Figure 3.** Binding energies of an electron bound to a hydrogenic impurity at the centre of inner QWW as a function of the outer QWWs thickness Lxa=Lxc for various electric field strengths.

In Fig. 3, the impurity is at the centre of inner wire. Unlike Fig. 2, the binding energy rapidly decreases about Lxa=Lxc $\approx$ 0.8a*. This is an expected behaviour. In the first, while the existence probability of the electron in inner wire is higher than outer wires, the existence probability of the electron in outer wires is increasing together with increasing outer wire thicknesses. Therefore, the binding energy shows rapid a decrease due to removing of the electron from the impurity.

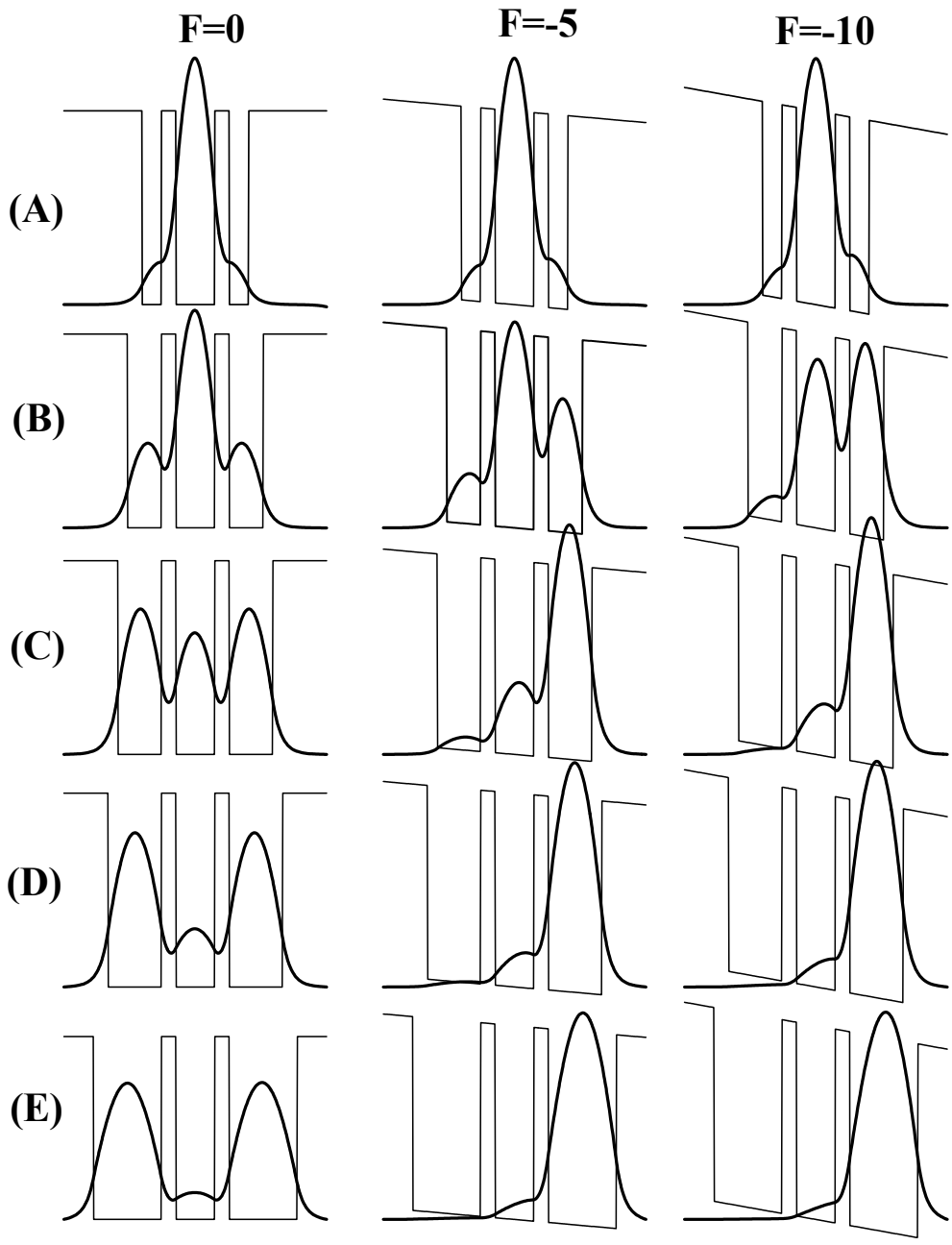


**Figure 4.** The electron distribution probability along the $x$ axis. For five different outer wire thicknesses (A:0.4a*, B:0.7a*, C:0.9a*, D:1.1a*, E:1.4a*) and three different electric field strengths.

The electron distribution probabilities have been shown in Fig. 4 for different outer wire thicknesses and electric field strengths. In this figure, Lxb=0.8a* and bra=brb=0.3a* are constants. For the zero electric field, the electron realises a transition from inner wire to outer wires as the outer wire thickness increases. This gives a reduction or increase in the probability of the finding the electron and impurity in the same plane. These tran-

sitions explain behaviour of rapid increase and decrease in the Figs 2-3**.** If the electric field is applied, the electron distribution probability is mostly confined to the right side of QWW.

In summary, we present numerically solved triple GaAs/$Al_xGa_{1-x}As$ QWWs for different cases. The results demonstrate that the binding energy of electron has changed with the electric field strength and the impurity position. It may particularly be useful in technological applications that the electron binding energy suddenly change with a small external electric field. In further studies the binding energy may also be investigated as a function of inner wire thickness, barrier thickness and electric field strength.

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