Qatar Univ. Sci. J. (1997), 17(2): 225-230

EFFECT OF ELECTRIC AND MAGNETIC FIELDS ON THE ENERGY LEVELS OF A HYDEROGENIC IMPURITY in GaAs/Ga1-xAlxAs HETROJUNCTIONS

M.I. El-Kawni and **K. F. Ilaiwi**

Department of Science Quds Open university
P.O. Box 893 Nablus — West bank

Department of Science Teacher's College of Education Ministry of Higher Education
P.O. Box 484, Code 411
Sur — Sultanate of Oman

استخدمت طريقة تقريبية للكتلة الفعالة لحساب حالات شغل الشوائب لعينات من زرنيخات الجاليوم والتي بها شوائب من الألومنيوم غير المتجانسة، كما استخدم دالة فنجر هولود كدالة تجريبية، ووجد المجال المغناطيسي والكهربائي المؤثر على طاقة ربط الشوائب في حالات التوزيع المتجانس والغير متجانس للحاجز.

Key Words : Hydrogenic impurity, GaAs/Gal-xAlxAs Heterojunctions.

ABSTRACT

Variational method within the effective — mass approximation is used to calculate the shallow impurities states in GaAs / $Ga_{1-x}Al_xAs$ heterojunctions. Modified Fang-Howard wavefunction is used as the trial wavefunction. Magnetic and electric fields effects on the impurity binding energy for the infinite and finite barrier heterojunctions are presented.

1. INTRODUCTION

Low-dimensional physical systems have always attracted considerable attention from both experimentalists and theorists.

The $GaAs/Ga_{1-x}Al_xAs$ heterojunctions is a well-studied example of these systems, in which regular band-gap variations, forming the superlattices, lead to the confinement of electrons and holes to well-defined regions in space [1-4]. The development of the molecular-beam-epitaxy technique together with the advancement made in the ultrahigh vaccum technology, achieving vaccum of less than 10^{-10} Torr, improved the experimental investigations in recent years.

From the theoretical point of view, much effort has also been done to understand the physical properties of these heterostructures [5-14]. For a complete discussion of various approaches to the problem of impurity states in inversion layers, the reader is referred to an excellent review by Ando et al. [15].

Originally, the infinite-barrier model is proposed to study the silicon and silicon dioxide, at the interface, where the potential height V_B is about 2eV. The Fang-Howard [16] wavefunction proposed for this model vanishes on the barrier, therefore, it is not acceptable for $GaAs/Ga_{1-x}Al_xAs$ case where the potential barrier height V_B is about 0.3eV.

The subject of low dimensional semiconductors, in presence of magnetic and electric fields has been a topic of great interest for along time. Bastard et al [17], report the effect of an external electric field on the eigenstates of Quantum well. Bastard et al [18], Sukumar et al [19], El-said et al [20], and Santigo et al [21], study the impurity ionization energies in static electric field. Green et al [22], Sukumar et al [23], and Peeters et al [24, 25], studies the impurity ionization in magnetic field. Moreover Ilaiwi et al [26], Ilaiwi [27, 28], and El-said et al [29], study the same problem in crossed electric and magnetic fields.

In this paper, the effects of electric and magnetic fields on shallow impurities in heterojunction have been studied, for the infinite and finite-barrier heterojunction, using the modifed Fang-Howard wavefunction which is acceptable for $GaAs/Ga_{1-x}Al_xAs$ This impurity wavefunction is allowed to penetrate the barrier region.

II.THEORY

The Hamiltonian describing the electron bound to the impurity at the interface in the presence of applied electric field and magnetic field B parallel to the growth axis and perpendicular to the interfaces can be written, within the framework of an effective mass approximation, as

$$H = H_o - \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) - \frac{2}{\varepsilon\,(x^2+y^2+z^2)^{1/2}} + \gamma L_z + \frac{1}{4}\gamma^2 (x^2+y^2)\,(Ry^*) \quad (1)$$

where,

$$H_o = -\mu \frac{\partial^2}{\partial z^2} + \frac{\delta}{z} + \eta z + V_B(z) \quad (2)$$

where μ-m_t^*/m_l^* is the ratio of the transversal to the longitudinal effective mass. u is equal to unity for the spherical energy ellipsoid corresponding to the conduction band of GaAs. The Colomb interaction is screened by background dielectric constant which is taken to be $\bar{\varepsilon} = (\varepsilon_1+\varepsilon_2)/2$. The term with $\delta = (\varepsilon_1+\varepsilon_2)/4\varepsilon_1$ where ε_1 is the dielectric constant of GaAs and ε_2 is the dielectric constant of $Ga_{1-x}Al_xAs$, describes the interaction of the electron with its image. $\eta = |e|\,a^*\,F$ is a measure of the electric field strenght and $\gamma = \hbar\omega_c/2$ (Ry*) with cyclotron frequency $\omega_c = e\,B/m^*c$ is used as the unit fo magnetic field. $V_B(z)$ in eq (2), the barrier potential of the interface, is defined as,

$$V_B(z) = \begin{cases} V_o\,, & z \le 0 \\ 0\,, & z \ge 0 \end{cases} \quad (3)$$

We have taken the barrier height to be

concentration dependent as it is related with the 60% rule, to the band gap difference ΔE_g of G*a*As and $Ga_{1-x}Al_xAs$. The band-gap difference has been determined from the following empirical expression [30];

$$\Delta E_g = 1.255x \quad \text{for } x \geq 0.3 \tag{4}$$

where x represent the concentration of Al.

Throughout our work the effective quantities $a^* = \hbar^2\bar{\varepsilon}/m^*e^2$ $Ry^* = m^*e^4/2\hbar^2\bar{\varepsilon^2}$ are used as the units of length and energy respectively.

The trial wavefunction proposed by Fang and Howard for Sri inversion layer is,

$$\psi_o = \left\{ \begin{matrix} 0 & , z \leq 0 \\ \sqrt{\frac{b_3}{2}} z \exp(-bz/2) & , z \geq 0 \end{matrix} \right\} \tag{5}$$

where b is the variational parameter. This wavefunction can be modified by allowing ψ_o to leak into the barrier to have the form,

$$\psi_o = \left\{ \begin{matrix} \exp(K_b z/2) & , z \leq 0 \\ (z+z_o)\exp(-bz/2) & , z \geq 0 \end{matrix} \right\} \tag{6}$$

Introducing the impurity wavefunction to be of the form $\psi(\vec{r}) = \psi(x,y)\ \psi_o$ where ψ_o is the modified Fang-Howard wavefunction given in eq. (6), the impurity trial wavefunction becomes,

$$\psi(\vec{r}) = \left\{ \begin{matrix} C \exp(K_b z/2) \exp(-a\rho/2) & , z \leq 0 \\ D(z+z_o)\exp(-bz/2)\ \exp(-a\rho/2), & z \geq 0 \end{matrix} \right\} \tag{7}$$

where
$\rho = (\chi^2+y^2)^{1/2}$, with $K_b = 2\sqrt{2m_2V_B/\hbar^2}$. The constants C, D, and z_o are found by using the continunity at Z = 0 and the normalization of the wavefunction. With this trial wavefunction, the γL_z term does not contribute to the expectation value and we have,

$$C = Dz_o \tag{8}$$

$$z_o = 2/(b + \kappa_b m_1/m_2) \tag{9}$$

$$D^2 = \left(\frac{a^2b^3\kappa_b}{2\pi} \right) [b^3z_0^2 + \kappa_b(2+2bz_0 + b^2z_0^2]^{-1} \tag{10}$$

In eq 7, a and b are used as variational parameters.
The impurity binding energy E_B is defined as [26],

$$E_B = E_S + \gamma - E_{2po} \tag{11}$$

where, E_s is the lowest subband energy defined as,

$$E_s = \frac{\langle \psi_o | H_o | \psi_o \rangle}{\langle \psi_o | \psi_o \rangle}, \tag{12}$$

E_{2po} is the eigenvalue of the Hamiltonian (1), defined by,

$$E_{2po} = \frac{\langle \psi(\vec{r}) | H | \psi(\vec{r}) \rangle}{\langle \psi(\vec{r}) | \psi(\vec{r}) \rangle}, \tag{13}$$

and γ is the energy of the first Landau level.

III. RESULTS AND CONCLUSIONS

By using the input parameters, x=0.3, V_o =226 meV, m_1=0.067m_o of G*a*As, m_2= (0.067 +0.06x) m_o = 0.085m_o of $Ga_{1-x}Al_xAs$, ε_1= 13.1 is the dielectric constant of G*a*As and ε_2=13.1 (1-x)+ 10.1x=12.2 is that for $Ga_{1-x}Al_xAs$, the impurity binding energy E_B has been calculated by using

equation (11).

The impurity binding energy E_B as a function of electric field strength F for infinite — barrier potential Heterostructures is considered in Figure 1, with different values of magnetic field γ , where γ =1 corresponds to a magnetic field of 67.4 kG. The impurity binding energies calculated in this figure, without the emagnetic field, are almost exactly the same as those found by Tomak and Godwin [9]. As shown in this Figure E_B is an ever increasing function of the electric field. This behaviour is understandable as an increasing filed piles up the wavefunction towards the interface where the impurity charge is present. The wavefunction cannot penetrate the barrier region and the electron feels the charge much better, it is also shown that, the binding energy increasing as the magnetic field increases as a result of increasing confinement.

This result is similar to those founded by Ilaiwi [28], for Infinite-barrier QW.

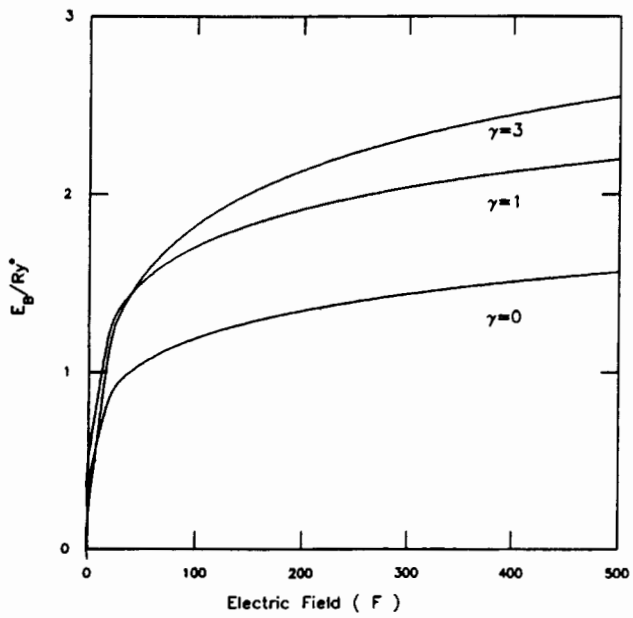

Figure 1.

Impurity binding energies E_B as a function of electric field strength F in $GaAs/Ga_{1-x}Al_xAs$ heterojunction for Infinite-barrier for different values of magnetic field.

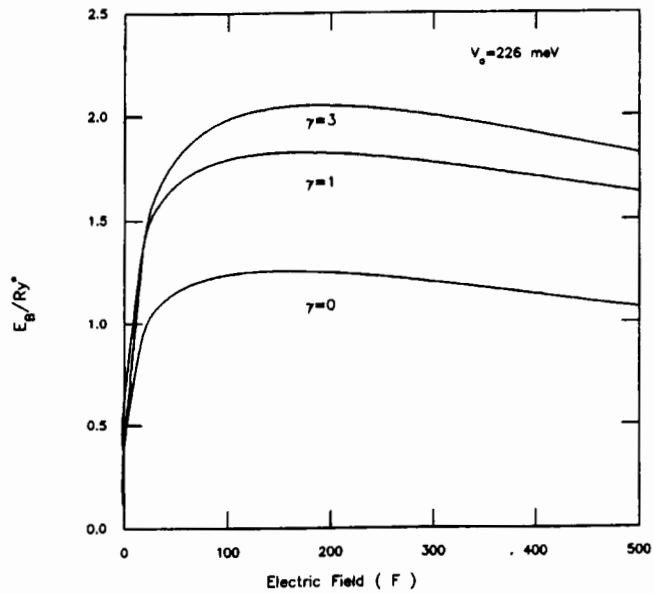

Figure 2.

Impurity binding energies E_B as a function of electric field strength F in $GaAs/Ga_{1-x}Al_xAs$ heterojunction for finite-barrier for different values of magnetic field.

The binding energy E_B as a function of electric field F for a finite-barrier potential V_o heterostructures is considered in Figure 2 for several values of magnetic field. As shown, the binding energy starts decreasing after an initial increase for smaller field values. This behaviour is expected as there is now a possibility for the electron to penetrate the barrier region and move away from the binding Coulomb center. This new feature is missisng in all previous calculations. Similar theoretical and experimental calculations for finite — barrier QW, are presented by shi et al [25], and Huant et al [31] respectively.

The new result presented in this paper for the finite-barrier should point out, however, that the anomalous regime where the binding starts to decrease again should be taken with caution, since the tunneling from such a state would be getting large in the same voltage range.

The impurity binding energy E_B as a function of magnetic field γ is presented in Figure 3 for finite — barrier case with two different values of

electric field. As seen from this figure, the binding energy E_B starts increasing as the magnetic field increases, but after a certain limit, E_B starts decreasing as magnetic field γ increase as a result of the possibility for the electron to penetrate the barrier region and move away from the binding Coulomb center.

There are, certainly, several points in this calculation that could be improved, Firstly, the form of variational wavefunction could be further modified to take into account the presence of the magnetic field better. This will also imporve the calculation of subband energy shift as a function of magnetic field. Secondly, no effort is made here for a better handling of the screeing effects. This could be done by using the r-dependent dielectric function instead of dielectric constant.

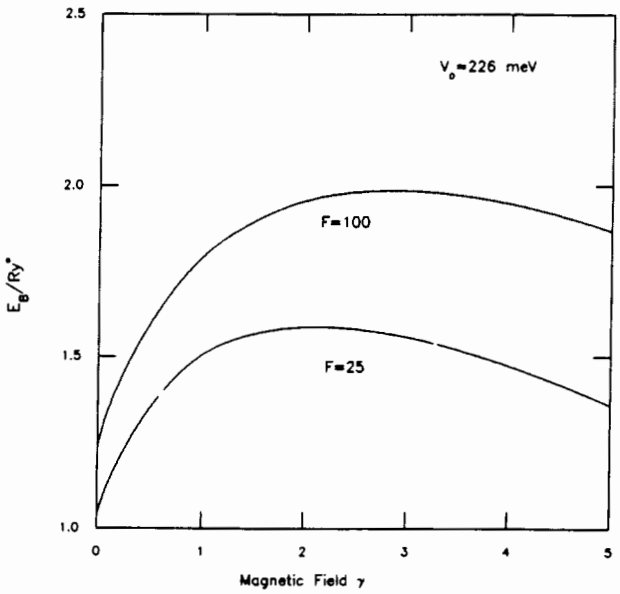

Figure 3.
Impurity binding energies E_B as function of magnetic field y in GaAs/$Ga_{1-x}Al_xAs$ heterojunction for finite-barrier for two different values of electric field.

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