Effects of hydrostatic pressure and magnetic field on donor binding energies in an inverse parabolic quantum well

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We compute the binding energy of donor hydrogenic impurities in a GaAs/GaAlAs inverse parabolic quantum well (IQPW), under hydrostatic pressure and a static magnetic field perpendicular to the well. The calculations were performed within the effective mass approximation using a variational approach. The binding energy was computed as a function of the impurity positions and quantum well widths. The result shows that an inverse parabolic quantum well turns into a parabolic quantum well with the effect of the magnetic field. Besides the binding energy increases with the pressure and magnetic field intensity, and the confinement is lost in a width which decreases with the pressure. We obtain that the profile inversion for the quantum well is associated with a minimum in the binding energy as function of the width of the well. Our results are in qualitative agreement with other theoretical works.

Keywords: Quantum well; inverse parabolic potential; binding energy.

1. Introduction

In recent years the theoretical studies and experimental results in nanotechnology have largely contribute to the development of this new technologies and have risen a great interest for the nanoscopic systems. The more commonly used structures for construction and study of this kind of systems are semiconductors, materials as GaAs, INP, SiGe, including alloys as GaAlAs, are the commonest.

Among the nanoscopic structures that have risen more interest in the last decade are the systems of low dimensionality: quantum wells, wires and dots have been some of the more studied for its optic properties and quantum effects.

The donor and acceptor type impurities as well as the treated excitons in this kind of nanodevices, have been study object during the last years, both theoretical and experimentally [1-11]. The impurities in semiconductor affect the optical and transport properties.

The first systems treated with hydrogenic impurities, were the quantum wells; there have done several works and studies with impurities in wells of different potential forms and in general, of different physics properties [1-4]. Furthermore there have studied the effects that produce on this kind of systems, parameters such as the magnetic field, the electric field, the hydrostatic pressure and others [1,4,13]. For example, the change in the binding energy of the impurity is one of those effects that gives many advantages when this type of nanodevices is manipulated.

2. The model

The system of study is an inverted parabolic quantum well of GaAs/Ga1−xAlxAs with a donor impurity, under the effects of a magnetic field and a hydrostatic pressure. The magnetic field is oriented perpendicular to the confinement direction [1], \( \vec{B} = (B, 0, 0) \).

The system hamiltonian, in the effective mass approximation in cgs units, is

\[
H = \frac{1}{2m^*_c(P)} \left[ \vec{p}^2 + e^2 \vec{A}(\vec{r}) \right] + v(z, P) - \frac{e^2}{e(P)r^2},
\]

where \( \vec{p} \) is the lineal momentum of the carrier and \( \vec{A} \) is the magnetic vector potential, \( m^*_c(p) \) is the effective mass of the electron in the material, \( e(P) \) is the dielectric constant and \( r' = (x^2 + y^2 + (z - r_d)^2)^{1/2} \) is the distance between the carrier and the impurity whose position along of the z axe is give by \( r_d \), placing the XY plane origin in the position of the impurity.

The confinement potential profile is

\[
V(z, P) = \begin{cases} 
\frac{V_d(P)}{\sigma} \left( 1 - \left( \frac{1}{L/P}\right)^2 \right)^2, & |z| \leq L/2 \\
V_b(P), & |z| > L/2 
\end{cases}
\]
where $\sigma = \chi_b/\chi_e$ is the ratio between the Al concentration at the barriers ($\chi_b$) and at the well center ($\chi_e$). $V_b(P)$ is the band discontinuity ($\chi_b = 0$; $3$) and $L(P)$ is the width of the well. The effective mass, the dielectric constant, the well’s width and the barrier height ($V_b(P)$) depend explicitly of the applied hydrostatic pressure. The hamiltonian in (1) can be written as

$$H = \frac{-\hbar^2}{2m^*_e(P)} \nabla_z^2 + \nu(z, P) - \frac{e^2}{\epsilon(P)r},$$

where $r = (x, y, z)$ is the carrier position vector and $\nu(z, P)$ is a effective potential given by

$$\nu = \frac{e^2B^2z^2}{2m^*_e(P)e^2} + V(z, P),$$

where we assume $\epsilon(0)=12.5$

Using a variational method, it’s chosen a typical test wave function,

$$\psi = B\chi(z)e^{-r''/\lambda},$$

where $r'' = \sqrt{x^2 + y^2}$ is a constant, $\chi(z)$ is the wave function that denotes the confinement in $z$ and $\lambda$ is the variational parameter. When the system energy is minimized, it’s found the impurity binding energy in the ground state,

$$E_b = E_1 - E_0,$$

$E_1$ is the energy of the ground state without impurities.

Taking advantage of the system symmetries, it can be write the Schrödinger equation using cylindrical coordinates.

$$\nabla^2\psi = (\nabla^2\chi)\xi + 2\nabla_z\chi\nabla_z\xi + \chi\nabla^2\xi.$$

On the other hand, the application of hydrostatic pressure modifies the lattice constant. The gap energy as function of the temperature in $K$ and the pressure in $kbar$ is [5]:

$$E_g^\Gamma = E_{g0} + \alpha P + \beta P^2 + b_1\frac{T^2}{T + c},$$

where $E_{g0}$ is the gap energy for $T=0$ and $P=0$, such that $E_{g0}(GaAs) = 1.519$ eV and

$$E_{g0}(Ga_{1-x}Al_xAs) = 1.519 + 1.155x + 0.37x^2 \text{ eV}.$$  

In the Eq. (5) $\alpha = 10.7$ meV/kbar and $\beta = -0.0377$ meV/kbar$^2$ inside the well; $\alpha = 1.5 - 1.3z$ meV/kbar and $\beta = 0$ outside the well, and $b_1 = 0.5405$ meV/K and $c = 204$ K both in the barriers and inside the well. The relations of the lattice constants with the pressure and the temperature are [2,6],

$$\frac{m^*_e(P, T)}{m_e} = \left[1 + E_P^\Gamma \left(\frac{2}{E_{g0}^\Gamma (P, T) + 1} + \frac{1}{E_g^\Gamma (P, T) + \Delta_0}\right)\right]$$

$$\epsilon(P, T) = \epsilon_0 e^{\delta_1(T - T_0) - \delta_2 P},$$

$$V(P, T) = 0.6\Delta E_g^\Gamma (P, T),$$

$$L(P) = L_0[1 - (S_{11} + 2S_{12})P],$$

where $E_P^\Gamma = 7.51$ eV, $\Delta_0 = 0.341$ eV, $\delta_1 = 9.4 \times 10^{-5} K^{-1}$, $\delta_2 = 1.67 \times 10^{-3} \text{kbar}^{-1}$, $T_0 = 75.6$ K, $S_{11} = -3.7 \times 10^{-4}$, $S_{12} = 1.16 \times 10^{-3}$ kbar$^{-1}$ and $\epsilon_0 = 12.5\epsilon_0$. $S_{11}$ and $S_{12}$ are the compliance constant of bulk GaAs [12] and $L_0$ is the IQPW width at $P=0$, and $\Delta E_g^\Gamma$ is the difference between Ga$_1$-$x$Al$_x$As and GaAs band-gaps at the point $\Gamma$.

3. Results and discussion

In the Fig. 1(a) the variation of the binding energy as a function of the impurity position for three values of magnetic field (B=0, B=15 T, y B=30 T) is shown, three values of $\sigma$ ($\sigma = 1$, $\sigma = 2$, $\sigma = 3$) and for a width of the well of 50 $\AA$. We observe a strong dependence with the Al concentration at center of inverted well and a not so strong dependence with the magnetic field. For the same value of $\sigma$, the electron confinement increases with magnetic field, and the increment of $x_c$ decreases the binding energy.

![Figure 1](image-url). Change in the impurity binding energy as function of the impurity position for three values of Al concentration at the center of well and magnetic field. P=0 and (a) L=50 $\AA$, (b) L=500 $\AA$.  

In the Fig. 1 (b), when L=500 Å, we note a strong dependence with the magnetic field unlike the case of L=50 Å. For B=0 is evident the inverted well effect, when the magnetic field is increased this effect is lost and it returns to a parabolic well. When B=15 T, there is a transition from IPQW to parabolic quantum well (PCW), and a small change in the concentration considerably affects the binding energy.

The results obtained in the Fig. 1(b) show binding energies higher than the obtained in the Ref. 1. This leads, according to the variational method, to a better approximation of the ground state energy. When the width of IPQW is considerably increased, the inverted well effects can be appreciated, under the necessity of large magnetic fields for obtain a parabolic well confinement.

The variation of the binding energy for B=0 and B=15 T, with $\sigma = 3$, L=50 Å and several values of hydrostatic pressure (P=0, P=20 kbar y P=30 kbar), as a function of the impurity position is shown in the Fig. 2(a). The presence of magnetic field increases the donor binding energy lightly. In contrast, the effect of hydrostatic pressure is considerable.

In all the cases the binding energies of impurity are of the order of MeV, expected values in quantum wells [2].

In the Fig. 2(b) with L=500 Å, it is observe the same behavior that the presented in the Fig. 1(b). Furthermore, the pressure increases the carrier confinement, however the increment in the binding energy is more sensitive to the magnetic field.

The behavior of the binding energy as function of the width of the well under the pressure effects and with $\sigma = 3$, is showed in the Fig. 3.

The binding energy increases from its bulk value as the width decreases, until the system reaches a values of critical width, then the energy drops to the bulk value of the barrier material as the width goes to zero.

We observe the hydrostatic pressure increases the binding energy, and the critical width that determine the peak decrease when the confinement is increased, in this case, in-
creasing the pressure. This result agrees with the known in the literature [2,4,8].

In the Fig. 4 the variation of the donor binding energy as a function of the IQPW width with magnetic field (B=15 T) is presented, for two different Al concentrations at the well center, and without the hydrostatic pressure effect. We observe that the binding energy decreases as the width increases, after of the critical L, as in the previous case, and later, due to the presence of magnetic field, the energy increases again, because of the inversion effect of the magnetic field. The critical width with $\sigma = 3$ is lightly lesser than in the case with $\sigma = 2$. Furthermore, the energy minimum caused by the presence of the magnetic field, is given in the case of $\sigma = 3$ (higher confinement) at a lesser L value (268 Å) than in the case of $\sigma = 2$ (295 Å) (lesser confinement), since with higher confinement, the width is lesser for which the inverted effects due to the magnetic field are appreciable.

4. Conclusions

We studied the behavior of the binding energy of a hydrogenic donor impurity immersed in an IPQW of GaAs/Ga$_{1-x}$Al$_x$As under the effects of pressure and magnetic field as function of the impurity position and the width of the well. We found that for values of the well width higher or equal to particular L the magnetic field inverts the IPQW effect. The binding energy increases with the magnetic field and the hydrostatic pressure.

Our results are in qualitative agreement with other theoretical works for quantum wells in presence of a magnetic field perpendicular to the well [1], taking into account the pressure effects without magnetic field [4,11], and taking into account the presence of pressure and magnetic field in parabolic quantum dots [10]. We obtain that the profile inversion for the quantum well is associated with a minimum in the binding energy as function of the width of the well, the width where the minimum is located is the lowest width value to obtain a parabolic quantum well as consequence of the magnetic field presence, that is a result that we don’t know has been reported previously.