Exciton Binding Energies in GaAs-$Al_{0.3}Ga_{0.7}As$ and $In_{0.53}Ga_{0.47}As$-InP Quantum Well Structures

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Abstract

The binding energies of the ground state of both the heavy-hole and light-hole excitons in a GaAs($In_{0.53}Ga_{0.47}As$) quantum well sandwiched between two semi-infinite $Al_{0.3}Ga_{0.7}As$(InP) layers are calculated as a function of well width in the presence of an arbitray magnetic field. A variational approach is followed using very simple trial wave function. The applied magnetic field is assumed to be parallel to the axis of growth and the binding energies are calculated for a finite value of the height of the potential barrier. The exciton binding energies for a given value of the magnetic field are found to be increased than their values in a zero magnetic field due to the compression of their wave functions within the well with the applied magnetic field.

I. Introduction

In recent years, the magnetic field effects on excitons in bulk and quantum wells have been extensively studied[1-4]. It is well known that external perturbations such as electric and magnetic fields may be used to understand the optical excitation spectra in solid[5]. The magnetic field is one of the most effective external perturbations for investigating the electronic band structure[2]. Since Green and Bajaj[1] first reported the exciton binding energies of *1s* state in GaAs-$Al_xGa_{1-x}As$ quantum well structures in the presence of the magnetic fields, several groups have attempted to measure the values of the binding energies of excitons in these quantum well systems[2, 3]. Green and Bajaj assumed that the valence subbands were decoupled and the applied field was parallel to the axis of growth. They find that for a given magnetic field, the binding energies are larger than their values in a zero field. In addition, the contribution to the binding energy due to the magnetic field, at a given field, increases slowly as the well size is reduced. Following their work, Yang and Sham[2] and Bauer and Ando[3] have calculated the binding energies of the *1s* states of excitons in quantum wells in the presence of a magnetic field including the valence subband coupling. Their results are very similar to those obtained by Green and Bajaj[1]. Recently, Cen and Bajaj[4] have reported the binding energies of excitons in a double quantum well in a magnetic field including the effects of subband mixing and also obtained the data for a single quantum well system to be compared with the results of Green and Bajaj. They find that for the case of the heavy hole, the exciton binding energy is in good agreement with the results of Green and Bajaj, but for the case of the light hole, their data are larger than those of Grren and Baja, who used 85-15% conduction-valence band offsets in their calculations, as light holes are more severely confined in quantum wells by higher potential barriers.

In this paper, a calculation of the binding energies of both heavy-hole and light-hole excitons in GaAs-$Al_{0.3}Ga_{0.7}As$ and lattice matched $In_{0.53}Ga_{0.47}As$-InP quantum well systems as a function of well size in the presence of an arbiturary magnetic field is presented. The methods reported in this paper can be applied to quantum well systems in which the electrons and holes are confined in the same semiconductor components and also have direct bandgap.

II. Theory

A carrier in a quantum well is confined within a one-dimensional potential well. The energy levels of such carriers are obtained by separating the system Hamiltonian into three parts, corresponding to the motion in the x, y, and z directions. When the thickness of the quantum well is comparable to the de Broglie wavelength, the kinetic energy corresponding to the carrier motion along the direction of confinement (assumed to be the z-axis) is quantized.

Fig. 1 shows a schematic diagram of the subband energy levels E_n of electrons and holes confined within a quantum well. The quantum well consists of the alternating $Al_xGa_{1-x}As$ (or InP)-GaAs (or $In_xGa_{1-x}As$)-$Al_xGa_{1-x}As$ (or InP) layer. The confined particle

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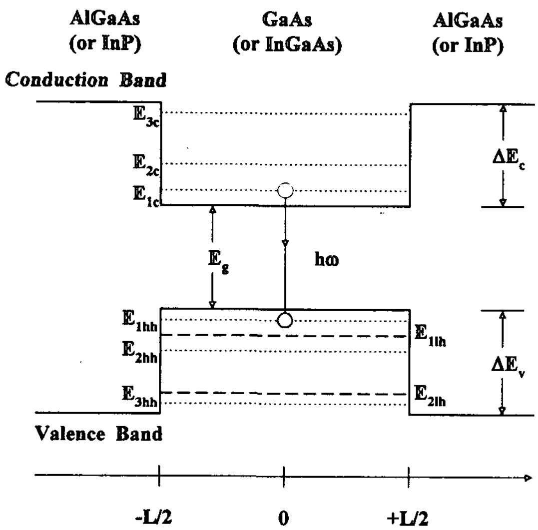

Fig. 1. Schematic diagram of the subband energy levels E_n of electrons and holes confined within a quantum well.

energy levels E_n are denoted by E_{1c}, E_{2c} and E_{3c} for electrons, by E_{1hh}, E_{2hh}, and E_{3hh} for heavy holes, and by E_{1lh} and E_{2lh} for light holes, respectively. In this paper the ground state wave functions and energies of E_{1c}, E_{1hh} and E_{1lh} are used to calculate the exciton binding energies.

In the presence of an external magnetic field, the Hamiltonian of an excitonic system in a GaAs ($In_{0.53}Ga_{0.47}As$) layer sandwiched between two semiinfinite layers of $Al_{0.3}Ga_{0.7}As$(InP) grown along the [001] direction can be given within the framework of an effective mass approximation[6], as

$$H_x = \frac{\hbar^2}{2m_e}\left(-i\nabla_e + \frac{e\vec{A}}{\hbar c}\right)^2 + \frac{\hbar^2}{2m_{\perp\pm}}(-i\nabla_z)^2 + \frac{\hbar^2}{2m_{\parallel\pm}}\left(-i\nabla_{\rho h} + \frac{e\vec{A}}{\hbar c}\right)^2 + V_e(z_e) + V_h(z_h) - \frac{e^2}{\varepsilon|\vec{r}|} \tag{1}$$

Here, $\vec{A}$ is the vector potential associated with the magnetic field $\vec{B}$, $m_{\perp\pm}$ is the effective mass of the heavy(+) or light(-) hole along the z-direction, and $m_{\parallel\pm}$ is the effective mass of the heavy(+) or light(-) hole in the x-y plane. The relative coordinate $\vec{r} = \vec{r_e} - \vec{r_h}$, where $\vec{r_e}$ and $\vec{r_h}$ are the position of the electron and hole, respectively. The potential wells for the conduction electron $V_e(z_e)$ and for the holes $V_h(z_h)$ are assumed to be square wells of width L and given by

$$V_e(z_e) = \begin{cases} 0, & |z_e| < L/2 \\ V_e, & |z_e| > L/2, \end{cases} \tag{2a}$$

$$V_h(z_h) = \begin{cases} 0, & |z_h| < L/2 \\ V_h, & |z_h| > L/2, \end{cases} \tag{2b}$$

For the GaAs-$Al_{0.3}Ga_{0.7}As$ system, V_e and V_h are determined from the Al concentration in $Al_xGa_{1-x}As$ using the following expression for the total band-gap discontinuity[7],

$$\Delta E_g = 1.155x + 0.37x^2 \tag{3}$$

in units of electron volts. The values of V_e and V_h are assumed to be 60% and 40% of ΔE_g, respectively. In the case of lattice-matched $In_{0.53}Ga_{0.47}As$-InP system, V_e=364.8 meV and V_h=243.2 meV are taken[8]. The trial envelope wave function for the exciton is chosen as

$$\Psi_x = f_e(z_e)g_h(z_h)R(\vec{\rho}) \tag{4}$$

where $f_e(z_e)$ and $g_h(z_h)$ are the normalized wave function for the electron and the hole, respectively, and $R(\vec{\rho})$ is the normalized envelope function in the x-y plane where the relative coordinate $\vec{\rho} = \vec{\rho_e} - \vec{\rho_h}$. This trial wave function satisfies the following effective-mass equation,

$$H_x\Psi_x = E\Psi_x \tag{5}$$

where E is the eigenvlaue of this equation. The vector potential $\vec{A}$ in cylindrical polar coordinates can be introduced as

$$\vec{A} = \frac{1}{2}\vec{B}\times\vec{r} \tag{6}$$

In this coordinate system, the envelope function $R(\vec{\rho})$ can be written by

$$R(\vec{\rho}) = \frac{1}{\sqrt{2\pi}}e^{im\Phi}G(\rho) \tag{7}$$

Here, m is the angular momentum to be zero for $1s$ state and $G(\rho)$ is the scalar envelope function given by

$$G(\rho) = N_\rho e^{-\delta\rho} \tag{8}$$

where N_ρ is the normalization factor and δ is a variational papameter which is adjusted to minimize the expectation value of the total energy. They are closely related to the exciton radius in a quantum well and have trends of increasing with decreasing well size until they reach their respective maxima and decreasing at rather small well size. The detail explanation for this is given later with the exciton binding energy as a function of well size.

Using the adiabatic approximation[9], the effective two dimen sional wave equation for a $1s$ state is given as

$$-\frac{\hbar^2}{2\mu_\pm}\left[\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}G(\rho)\right] + \left[\frac{\mu_\pm}{8}\omega_H^2\rho^2 + V(\rho)\right]G(\rho) = E_xG(\rho) \tag{9}$$

where $\mu_\pm$ is the reduced mass corresponding to heavy hole(+) or light hole(-) bands in the x-y plane given by

$$\frac{1}{\mu_\pm} = \frac{1}{m_e} + \frac{1}{m_0}(\gamma_1 \pm \gamma_2) \quad (10)$$

Here, m_e is the effective mass of the conduction electron and m_0 is the free electron mass, and γ_1 and γ_2 are the material parameters[6] which are related to valence band structure. For a GaAs-$Al_{0.3}Ga_{0.7}As$ quantum well, ε =12.5, m_e=0.067m_0, γ_1=6.93, and γ_2=2.15[1] (for a lattice matched $In_{0.53}Ga_{0.47}As$-InP quantum well structure, ε =13.56, m_e=0.0437m_0, γ_1=13.7, and γ_2=5.47[8]) are adopted. Also, $V(\rho)$ in Eq. (9) is the effective two dimensional Coulomb potential defined as

$$V(\rho) = -\frac{e^2}{\varepsilon}\int\int \frac{|f_e(z_e)|^2 \cdot |g_h(z_h)|^2}{|\vec{r}|} dz_e dz_h \quad (11)$$

ω_H is the cyclotron frequency given by

$$\omega_H = \frac{eB}{\mu_\pm c} \quad (12)$$

where B is the magnitude of the applied magnetic field and c is the speed of light in vacuum. E_x, the eigen value of this wave equation, is given by

$$E_x = E - E_e - E_h \quad (13)$$

where E_e and E_h are the ground state subband energies of the electron and hole, respectively, which are obtained by numerically solving the transcendental equations given by

$$\left[\frac{E_e}{V_e}\right]^{1/2} = \cos\left[\frac{m_e E_e}{2\hbar^2} L\right]^{1/2} \quad (14a)$$

$$\left[\frac{E_h}{V_h}\right]^{1/2} = \cos\left[\frac{m_{\perp\pm} E_h}{2\hbar^2} L\right]^{1/2} \quad (14b)$$

The binding energy of the ground state, E_B can then be expressed as

$$E_B = E'_e + E'_h - \langle E_x \rangle \quad (15)$$

where $\langle E_x \rangle$ is obtained by evaluating the expectation value of H_x variationally. E'_e and E'_h, the new ground state subband energies of the electron and hole, respectively, due to the magnetic field, are given by

$$E'_e = E_e + e\frac{\hbar B}{2m_e c} \quad (16a)$$

$$E'_h = E_h + e\frac{\hbar B}{2m_{\perp\pm} c} \quad (16b)$$

III. Results and Discussion

We have calculated the values of the binding energies of the ground state of the heavy-hole and the light-hole exciton in a lattice-matched GaAs-$Al_{0.3}Ga_{0.7}As$($In_{0.53}Ga_{0.47}As$-InP) quantum well structure as a function of well width for several values of the magnetic field.

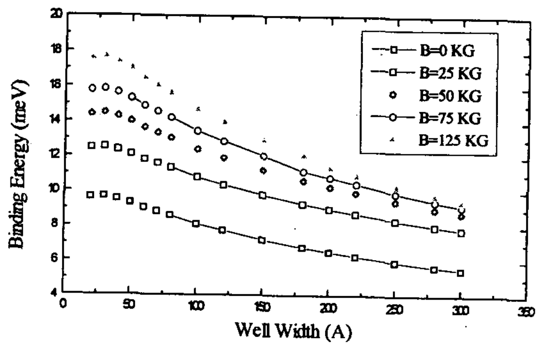

Fig. 2. The binding energy of the heavy hole exciton as a function of well width in GaAs-$Al_{0.3}Ga_{0.7}As$ quantum wells for several magnetic fields.

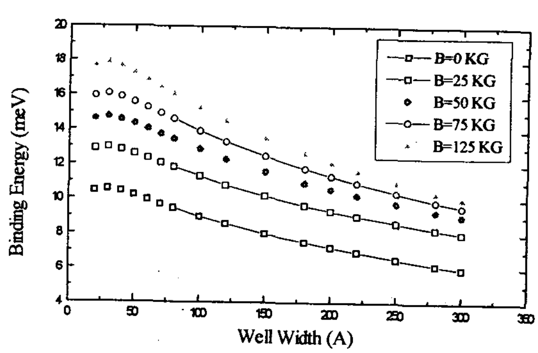

Fig. 3. The binding energy of the light hole exciton as a function of well width in GaAs-$Al_{0.3}Ga_{0.7}As$ quantum wells for several magnetic fields.

Figs. 2 and 3 show the heavy- and light-hole exciton binding energy for a GaAs-$Al_{0.3}Ga_{0.7}As$ quantum well, respectively and Figs. 4 and 5 for a $In_{0.53}Ga_{0.47}As$-InP quantum well, respectively. As far as we know this is the first reported attempt to determine the exciton binding energies in the presence of magnetic fields for $In_{0.53}Ga_{0.47}As$-InP quantum well system. For comparison, we also show the variations of both heavy-hole and the light-hole binding energies with well size for zero magnetic field.

From the figures, the binding energies of the heavy-hole and the light-hole excitons increase with increasing magnetic field. The reason for these results is that in the presence of a magnetic field, the exciton in a quantum well is more compressed and its binding energy is more increased than that of the zero magnetic field.

Furthermore, for a given magnetic field (or zero magnetic field), both exciton binding energies increase as well size is reduced until they reach their respective maxima, and then decrease again. The reason is that for wide wells the exciton wave function is compressed in the quantum well leading to increasing binding

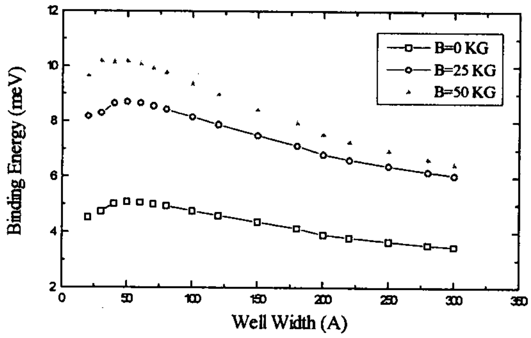

Fig. 4. The binding energy of the heavy hole exciton as a function of well width in $In_{0.53}Ga_{0.47}As$-InP quantum wells for several magnetic fields.

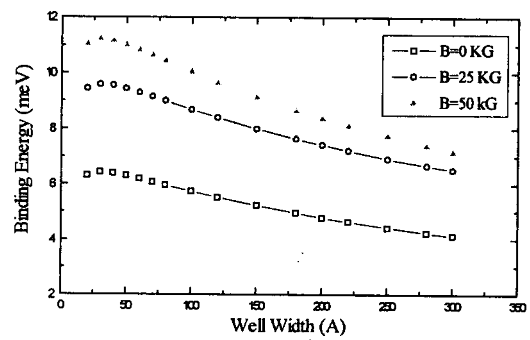

Fig. 5. The binding energy of the light hole exciton as a function of well width in $In_{0.53}Ga_{0.47}As$-InP quantum wells for several magnetic fields.

with decreasing well size. However, below a certain value of well size, the spread of the exciton wave function into the surrounding AlGaAs(InP) layers becomes more important, thus reducing the effective Coulomb attraction and therefore binding energies. In Figs. 2 and 3, we find that for a $GaAs$-$Al_{0.3}Ga_{0.7}As$ quantum well structure, the exciton binding energies of the heavy- and light-hole in a high magnetic field (B=125 KG) behave differently. This is because our envelope function is rather simple and is not quite appropriate in the high field case.

For the case of a $In_{0.53}Ga_{0.47}As$-InP quantum well in Figs. 4 and 5, the variation of exciton binding energies of the heavy- and light-hole with well width at B=50 KG is different than at lower fields. Since the effective mass of the hole ($\mu_{\pm}$) in a $In_{0.53}Ga_{0.47}As$-InP quantum well are smaller than those in a $GaAs$-$Al_{0.3}Ga_{0.7}As$ quantum well, the exciton binding energies of the former are smaller than those of the latter. Therefore, the variation of the exciton binding energies in a $In_{0.53}Ga_{0.47}As$-InP quantum well deviates at lesser fields than that in a $GaAs$-$Al_{0.3}Ga_{0.7}As$ quantum well.

For the case of a $GaAs$-$Al_{0.3}Ga_{0.7}As$ quantum well structure, our data are compared with those of Cen and Bajaj[4], who calculated the binding energies of heavy- and light-hole excitons

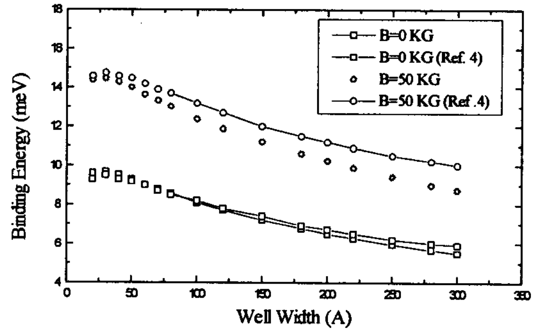

Fig. 6. The binding energy of the heavy hole exciton as a function of well width in $GaAs$-$Al_{0.3}Ga_{0.7}As$ quantum wells for B=0 KG and B= 50 KG. The solid square(□) and solid circle(○) are our results with subband decoupled; The open square(□) and open circle(○) are by Cen and Bajaj (Ref. 4) with subband mixing.

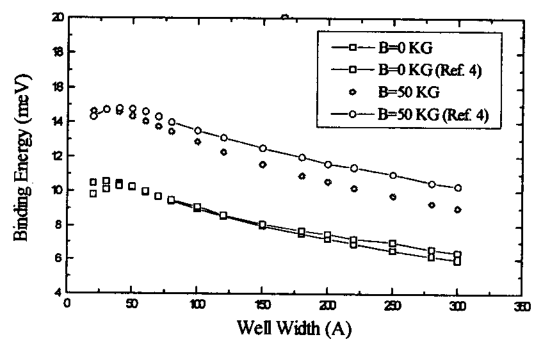

Fig. 7. The binding energy of the light hole exciton as a function of well width in $GaAs$-$Al_{0.3}Ga_{0.7}As$ quantum wells for B=0 KG and B= 50 KG. The solid square(□) and solid circle(○) are our results with subband decoupled; The open square(□) and open circle(○) are by Cen and Bajaj (Ref. 4) with subband mixing.

in GaAs-AlGaAs double quantum well systems including subband mixing effects. They also show the data for the single quantum well with the same approach and these results are shown in Figs. 6 and 7 for the heavy-hole and light-hole excitons, respectively. Even though we have used a quite simple trial wave function [Eq. (8)], our results are very close to those of ref. 4 for B=0 KG and a little lower than those of ref. 4 with increasing well width for B=50 KG, because we have neglected contribution of the subband mixing effects, whereas they included these effects to calculate the exciton binding energies.

Ⅳ. Summary

In this paper, using the variational approach, the binding energies of the ground state of both the heavy-hole and light-hole excitons in a $GaAs$-$Al_{0.3}Ga_{0.7}As$ and a $In_{0.53}Ga_{0.47}As$-InP quantum well system have been calculated as a function of well width with the applied magnetic field. The exciton binding energies for both a $GaAs\text{-}Al_{0.3}Ga_{0.7}As$ and a $In_{0.53}Ga_{0.47}As\text{-}InP$ quantum well systems for a given value of the magnetic field are found to be increased than their values in a zero magnetic field due to the compression of their wave functions within the well with a magnetic field. Also, the exciton binding energies of the both GaAs-AlGaAs and InGaAs-InP quantum well systems are decreased with increasing well size for a given magnetic field and for the moderate well width. Even though a very simple trial wave function is used for the calculation, our results for a $GaAs\text{-}Al_{0.3}Ga_{0.7}As$ quantum well system are in good agreement with those of others. For the case of a $In_{0.53}Ga_{0.47}As\text{-}InP$ quantum well system, this calculation is the first reported attempt to determine the exciton binding energies as a function of well width with and without applied magnetic fields. The exciton binding energies in $In_{0.53}Ga_{0.47}As\text{-}InP$ quantum wells are smaller than those in GaAs-AlGaAs quantum wells due to their smaller effective mass of the hole compared to that of the latter. These results can be used to characterize optical properties of compound semiconductors which have quantum well structures.

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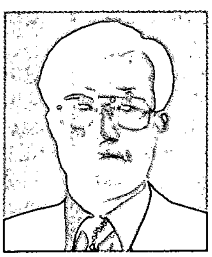

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