# Optical Properties of an Exciton in Quantum Well Structures

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## Abstract

In this paper, the oscillator strengths of both the heavy-hole and the light-hole excitons in GaAs-$A_{l0.3}Ga_{0.7}As$ and $In_{0.53}Ga_{0.47}As$-InP quantum wells with the effect of a magnetic field applied along the growth axis are studied. The calculation is carried out using a variational approach, based on a simple trial exciton wave function. The exciton oscillator strengths are found to decrease with increasing well width and to increase with the applied magnetic fields which lead to additional quantum confinement for moderately wide well sizes. Also, the oscillator strengths for the heavy-hole exciton are found to be larger than those of the light-hole exciton in these quantum well structures.

## I. Introduction

There has been a great deal of interest in investigating the optical properties of quantum well structures including both photoluminescence and absorption spectra [1-3]. It is well known that external perturbations such as electric and magnetic fields may be used to understand the optical excitation spectra in solid [4]. The magnetic field is one of the most effective external perturbations for investigating the electronic band structure and properties of quantum wells [5]. Recently, emission and absorption spectra associated with both the heavy-hole and the light-hole excitons in the presence of a magnetic field have been observed in heterostructure quantum well systems [6,7]. Many of these experiments are motivated by the fact that there is a steadily increasing number of technological applications for the optoelectronic properties of quantum wells [8]. The oscillator strength is the quantity which describes the probability of a quantum mechanical transition between two states [9]. Also, it is well known to be closely related with the exciton peaks at the absorption edges of each of the subband to subband transitions.

The work on the oscillator strength in quantum wells has been done both theoretically and experimentally [10-12]. Brum and Bastard [10] calculated the oscillator strengths $f_{n,m}$ of the *(n,m)* excitonic transition as a function of well width, where *n (m)* labels the electron (hole) subbands in a GaAs-$Al_{0.3}Ga_{0.7}As$ quantum well. They find that the *n=0* excitonic transitions are stronger than others and that the heavy-hole $f_{n,m}$ is larger than the light-hole $f_{n,m}$. Sanders and Chang [11] also calculated the oscillator strengths for several prominent excitons in a GaAs- $Al_{0.25}Ga_{0.75}As$ quantum well with the variation of well width taking into account the effects of valence-band hybridization. They find that the exciton oscillator strengths have a trend of decreasing with well width for moderately wide wells, on account of wave-function spreading as Brum and Bastard [10] obtained. Their calculation for the oscillator strengths are in qualitative agreement with the experiments [12].

In this paper, exciton oscillator strengths in both GaAs-$Al_{0.3}Ga_{0.7}As$ and $In_{0.53}Ga_{0.47}As$-InP quantum well structures with the effect of applied magnetic field are calculated and discussed.

## II. Theory

In our model, we assume that the magnetic field is applied parallel to the direction of growth [001] of the quantum well structure. Also, only the excitons with allowed transition ($\Delta n=0$) are considered in this paper.

The exciton oscillator strength, $f_{n,m}$ for an optical transition from a valence band state *m* to a conduction band state *n* is obtained using Fermi's Golden rule and is given by [13]

$$f_{n,m}=\frac{2}{E_g m_0}\left|\sum_{k}\Psi_{n,m}(\vec{k})\cdot\hat{\varepsilon}\cdot\vec{P}_{n,m}(\vec{k})\right|^2 \qquad (1)$$

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where $m_0$ is the free electron mass, $E_g$ is the band gap (*1.52 eV*) in bulk GaAs (*0.812 eV* for $In_{0.53}Ga_{0.47}As$), $\Psi_{n,m}(\vec{k})$ is the exciton-relative-motion envelope function in $k$ space and given by

$$\Psi_{n,m}(\vec{k}) = f_n(z_e) g_m(z_h) G_{n,m}(\rho, z, \phi) \tag{2}$$

Where $z = z_e - z_h$, $f_n(z_e)$ and $g_m(z_h)$ are the well-known ground state solutions of the finite square well problem for electron and hole, respectively. The wave function $G_{n,m}(\rho, z, \phi)$ describes the internal motion of the exciton. In this paper, the following simple form for this trial wave function is chosen [7,10].

$$G_{n,m}(\rho, z, \phi) = N_\rho e^{-\delta\rho} \tag{3}$$

Here, $N_\rho$ is the normalization factor and $\delta$ is a variational parameter which is adjusted to minimize the expectation value of the total energy. This wave function is believed to be the simplest form that can be chosen while still preserving the principal features of the actual wave function in a quantum well. Note that any $\Psi_{n,m}(\vec{k})$ is orthogonal to all the $\Psi_{n',m'}(\vec{k})$ with $(n',m') \neq (n,m)$. This warrants that the expectation values of exciton Hamiltonian, $H$ over $\Psi_{n,m}(\vec{k})$ will always be lower bounds to the true exciton binding energies [10]. $\hat{\varepsilon}$ is the polarization vector and $\vec{P}_{n,m}(\vec{k})$ is the optical matrix element between two Bloch states. Here the optical matrix element is given by

$$\vec{P}_{n,m}(\vec{k}) = \langle \Psi^h_m | \vec{P} | \Psi^e_n \rangle \tag{4}$$

where $\Psi^h_m(\vec{k})$ and $\Psi^e_n(\vec{k})$ are the valence and conduction subband wave fuctions, respectively and satisfies the following effective-mass equation,

$$H\Psi = E\Psi \tag{5}$$

where $E$ is the eigenvalue of this equation and the Hamiltonian of an excitonic system in our system in the presence of an external magnetic field can be given by [14]

$$H = \frac{\hbar^2}{2m_e}\left(-i\vec{\nabla}_e + \frac{e\vec{A}}{\hbar c}\right)^2 + \frac{\hbar^2}{2m_{\perp\pm}}(-i\vec{\nabla}_z)^2 + \frac{\hbar^2}{2m_{\parallel\pm}}\left(-i\vec{\nabla}_{\rho h} + \frac{e\vec{A}}{\hbar c}\right)^2 \\ V_e(z_e) + V_h(z_h) - \frac{e^2}{\varepsilon|\vec{r}|} \tag{6}$$

Here $\vec{A}$ is the vector potential associated with the magnetic field $\vec{B}$, $m_e$ is the effective mass of the conduction band electron, $m_{\perp\pm}$ is the heavy(+) or light(-) hole mass along the $z$-direction, and $m_{\parallel\pm}$ is the effective mass of the heavy(+) or light(-) hole in the $x$-$y$ plane, which are given by $1/m_{\perp\pm} = \gamma_1 \mp 2\gamma_2$ and $1/m_{\parallel\pm} = \gamma_1 \pm \gamma_2$, respectively. For a $GaAs$-$Al_{0.3}Ga_{0.7}As$ quantum well, $\varepsilon = 12.5$, $m_e = 0.067m_0$, Luttinger parameters, $\gamma_1 = 6.93$ and $\gamma_2 = 2.15$ [15] (for a lattice matched $In_{0.53}Ga_{0.47}As$-InP quantum well case, $\varepsilon = 13.56$, $m_e = 0.0437m_0$, $\gamma_1 = 13.7$, and $\gamma_2 = 5.47$) [16] are adopted. $V_e(z_e)$ and $V_h(z_h)$ are the square potential wells for the conduction electron and the valence holes, respectively and their potential heights are determined from *Al* concentration in $GaAs$-$Al_xGa_{1-x}As$ quantum well system, using the expression for the total-bandgap discontinuity [17], $\Delta E_g = (1.155x + 0.37x^2)$ in units of electron volts. In this paper, $x = 0.3$ for the $GaAs$-$Al_xGa_{1-x}As$ quantum wells is used and the values of $V_e$ and $V_h$ are assumed to be *60%* and *40%* of $\Delta E_g$, respectively. (In the case of lattice matched $In_{0.53}Ga_{0.47}As$-InP quantum wells, $V_e$=364.8 *meV* and $V_h$=243.2 *meV* are taken [16] ). In the envelope function approximation for the eq. (2),

$$\Psi^h_m(\vec{k}) = \sum_v g^v_m(\vec{k}, z) e^{i\vec{k}\cdot\vec{\rho}} \mid \Psi^h_v\rangle \tag{7.a}$$

$$\Psi^e_n(\vec{k}) = \sum_\sigma f^\sigma_n(\vec{k}, z) e^{i\vec{k}\cdot\vec{\rho}} \mid \Psi^e_\sigma\rangle \tag{7.b}$$

where the hole spin $\nu$ = -3/2, -1/2, +1/2, +3/2 and the electron spin $\sigma$ = -1/2, +1/2. The corresponding hole and electron envelope functions are $g^v_m(\vec{k}, z)$ and $f^\sigma_n(\vec{k}, z)$, respectively and the zone center Bloch functions for electrons and holes are $\mid \Psi^e_\sigma\rangle$ and $\mid \Psi^h_v\rangle$, respectively.

Then, the expression for the optical matrix element becomes

$$\hat{\varepsilon}\cdot\vec{P}_{nm}(\vec{k}) = \sum_{v,\sigma} \langle g^v_m \mid f^\sigma_n\rangle\langle \Psi^h_v | \hat{\varepsilon}\cdot\vec{P} | \Psi^e_\sigma\rangle \tag{8}$$

Here, $\langle \Psi^h_\nu | \hat{\varepsilon}\cdot\vec{P} | \Psi^e_\sigma\rangle$ are the non vanishing bulk optical matrix elements and given by [13]

$$\left\langle \pm\frac{3}{2} | P_x | \pm\frac{1}{2} \right\rangle = \frac{1}{\sqrt{2}} \langle s | P_x | x\rangle \tag{9.a}$$

$$\left\langle \pm\frac{1}{2} | P_x | \pm\frac{1}{2} \right\rangle = \frac{1}{\sqrt{6}} \langle s | P_x | x\rangle \tag{9.b}$$

where the matrix element $\langle s | P_x | x\rangle$ is a constant defined in ref. 16. For example, the values of the squared momentum matrix are *25.7* and *20.4 eV* for GaAs and InP, respectively. For the model used in this paper, the $k$-dependence of $\vec{P}_{n,m}(\vec{k})$ is neglected and the equation reduced to

$$f_{n,m} = \frac{2}{E_g m_0} |\hat{\varepsilon}\cdot\vec{P}_{n,m}(\vec{k}=0)|^2 \cdot |G_{n,m}(\vec{\rho}=0)|^2 \tag{10}$$

Since the direction of polarization is perpendicular to the $z$-direction when unpolarized light is incident along the [001] growth direction, equation (10) becomes

$$f_{n,m} = \frac{2}{E_g m_0} |\hat{x}\cdot\vec{P}|^2 \cdot |G_{n,m}(\vec{\rho}=0)|^2 \tag{11}$$

Then, the oscllator strength $f_{n,m}$ is proportional to $|G(\vec{\rho}=0)|^2$ since it is proportional to the probability that electrons and holes are in the same unit cell.

## III. Results and Discussion

The oscillator strengths per unit area, $f_{1,1}(10^{-5}, \text{Å}^{-2})$ are calculated within the two-band exciton model as a function of well width with and without applied magnetic fields and shown in Figs. 1 and 2 for GaAs-Al$_{0.3}$Ga$_{0.7}$As quantum wells and in Figs. 3 and 4 for In$_{0.53}$Ga$_{0.47}$As-InP quantum wells.

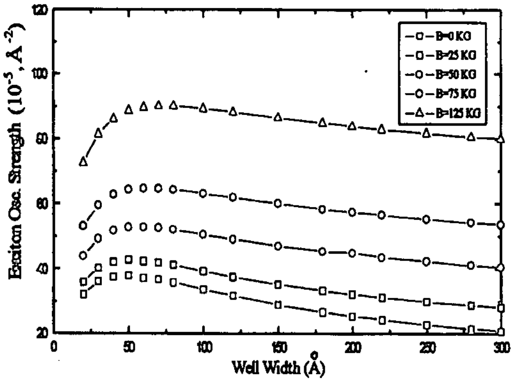

**Fig. 1.** Oscillator strengths of the heavy-hole exciton per unit area as a function of well width in GaAs-Al$_{0.3}$ Ga$_{0.7}$As quantum wells for several magnetic fields.

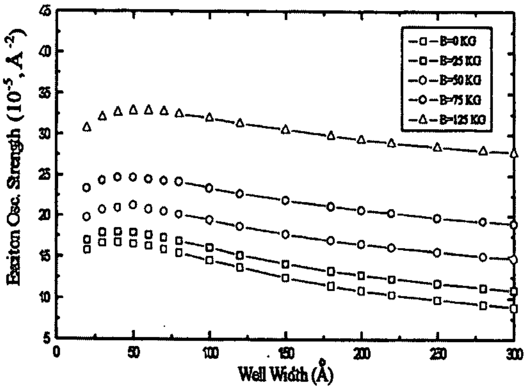

**Fig. 2.** Oscillator strengths of the light-hole exciton per unit area as a function of well width in GaAs-Ai$_{0.3}$ Ga$_{0.7}$As quantum wells for several magnetic fields.

From the figures, the exciton oscillator strengths are found to decrease with increasing well width for moderately wide wells, on account of wave function spreading. But for narrow wells, it decreases after it reaches a maximum as well width is reduced. The wave functions tend to spill over into the surrounding Al$_{0.3}$Ga$_{0.7}$As (InP) layers with decreasing well size and these effects are significant for narrow wells. Therefore, exciton binding energies [18] and then oscillator strengths begin to fall off rather rapidly in these range. Also, we find that the oscillator strengths for the heavy-hole exciton are larger than those of the light-hole exciton. This is because the values of the optical matrix element of the heavy-hole are much larger than those of the light-hole in eq. (11) even though the value of $|G(\vec{\rho}=0)|^2$ of the former case is a little smaller than that of the latter.

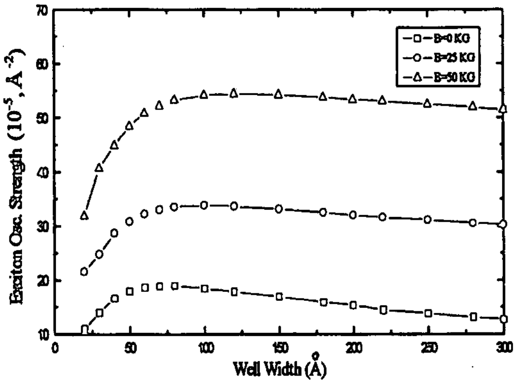

**Fig. 3.** Oscillator strengths of the heavy-hole exciton per unit area as a function of well width in In$_{0.53}$Ga$_{0.47}$As-InP quantum wells for several magnetic fields.

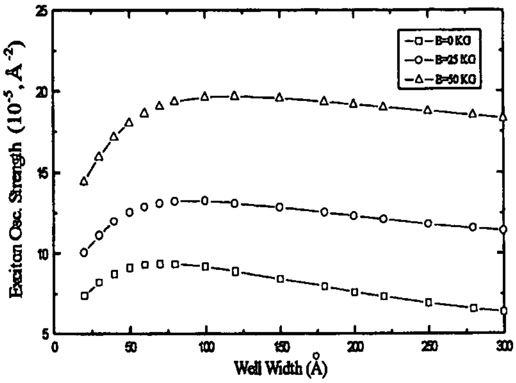

**Fig. 4.** Oscillator strengths of the light-hole exciton per unit area as a function of well width in In$_{0.53}$Ga$_{0.47}$As-InP quantum wells for several magnetic fields.

Also, it is seen that the oscillator strengths of the heavy-hole and the light-hole excitons for both quantum well systems increase as the applied magnetic field increases. This can be explained as follows. As the magnetic field increases, the exciton wave functions are more compressed within the well and the value of $|G(\vec{\rho}=0)|^2$ is also increased. As explained before, since the exciton oscillator strength is proportional to $|G(\vec{\rho}=0)|^2$, the exciton oscillator strength $f_{1,1}$ is increased with increasing magnetic field.

To check the accuracy of our trial wave function we have calculated the values of binding energies of the heavy-hole exciton and the light-hole exciton as a function of well width for several values of the magnetic field [19]. The calculated values of the exciton binding energies are very close to those obtained by Cen and Bajaj [18] using a more elaborate form of the trial wave function. Also, for the case of GaAs-$Al_{0.3}Ga_{0.7}As$ quantum well structures, our results for the exciton oscillator strengths for *B=0 KG* can be compared with the data by Sanders and Chang [11] and experimental one by Voliotis, *et. al.* [20]. These results are shown in Figs. 5 and 6 for the heavy-hole and the light-hole excitons, respectively.

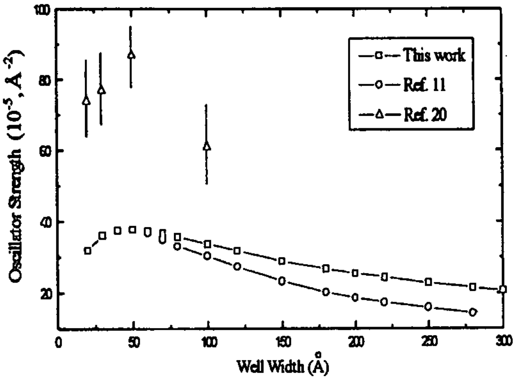

**Fig. 5.** Comparison of calculated and measured values of the oscillator strengths for the heavy-hole exciton in a GaAs-AlGaAs quantum well. The soild square(☐) is our results; solid circle(○) is calculated by Sanders and Chang (Ref. 11); solid triangle(△) is experimental data by Voliotis, et. al.(Ref. 20)

Our data are found to be close to but a little higher than those of Sanders and Chang with increasing well size. This is because while we used quite simple trial wave function, they employed the complicated wave function as the sum of nine Gaussians with exponents to cover a broad physical range. Also, the exciton oscillator strength is very sensitive to the wave function. Therefore, as the well size increases, their wave function is more suffered from spreading effect than ours. Experimental data by Voliotis, *et. al.* [20] is obtained by the absorption spectra. They caculated exciton oscillator strength per unit area from the integrated absorption over the exciton peak. As they stated in that paper, these experimental data include some error specially for wide well. As it can be seen in the figures, the experimental results are almost twice as large as the calculated results of the oscillator strengths by ours and by Sanders and Chang. This may be due to the difference in definition of the oscillator strength between the theoretically calculated and the experimental data. Note that the ratio of the oscillator strength between the lighty-hole exciton and the heavyt-hole exciton is almost 2.

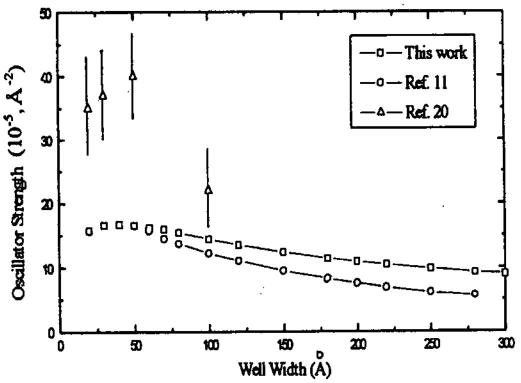

**Fig. 6.** Comparison of calculated and measured values of the oscillator strengths for the light-hole exciton in a GaAs-AlGaAs quantum well. The soild square(☐) is our results; solid circle(○) is calculated by Sanders and Chang (Ref. 11); solid triangle(△) is experimental data by Voliotis, et. al.(Ref. 20)

For the $In_{0.53}Ga_{0.47}As$-InP quantum wells, this is the first reported attempt to calculate the exciton oscillator strengths with the effects of the applied magnetic fields in this system. From the figures, the variations of the oscillator strengths of both the heavy-hole and the light-hole excitons with the applied magnetic field in the $In_{0.53}Ga_{0.47}As$-InP quantum wells are shown up to *B=50 KG* while those data in GaAs-$Al_{0.3}Ga_{0.7}As$ quantum well structures are shown up to *B=125 KG*. We find the exciton binding energies and thus the oscillator strengths of both quantum well systems behave differently in high magnetic fields (*B≥50 KG* and *B≥125 KG* in $In_{0.53}Ga_{0.47}As$-InP and GaAs-$Al_{0.3}Ga_{0.7}As$ quantum wells, respectively). Theses results are believed that our envelope function is rather simple and is not quite appropriate in the high field case. Since the effective mass of the electron and the hole, and reduced mass of the hole 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 former has the smaller value of $|G(\vec{\rho}=0)|^2$ than the latter. That means $In_{0.53}Ga_{0.47}$ As-InP quantum wells have the smaller variational parameter for a given well width, which is closely related to the exciton extent in the *x-y* plane, than GaAs-$Al_{0.3}Ga_{0.7}As$ quantum wells. Therefore, the exciton oscillator strengths of the $In_{0.53}Ga_{0.47}As$-InP quantum wells are smaller than those of GaAs-$Al_{0.3}Ga_{0.7}As$ quantum wells.

## IV. Summary

We have calculated the oscillator strengths of the heavy-hole and the light-hole excitons per unit area as a function of well width in GaAs-$Al_{0.3}Ga_{0.7}As$ and $In_{0.53}Ga_{0.47}As$-InP quantum well systems with and without the applied magnetic fields. For the moderate well size, the exciton oscillator strengths have been found to decrease with increasing well width and increase with increasing applied magnetic field. Even though a simple trial wave function for the exciton in quantum wells has been used to the calculation, the results for the case of the GaAs-$Al_{0.3}Ga_{0.7}As$ quantum wells with $B=0$ *KG* are in good agreement with others, while the calculated data are less almost factor 2 than the experimental one. Therefore, the exciton oscillator strengths per unit area with the perturbations such as external magnetic fields in GaAs-AlGaAs and InGaAs-InP quantum well systems are believed to be determined reasonably by the methods suggested in this paper.

For the $In_{0.53}Ga_{0.47}As$-InP quantum well systems, this is the first reported attempt to calculate the exciton oscillator strengths with and without the applied magnetic filed. The exciton oscillator strengths of the heavy-hole and the light-hole in $In_{0.53}Ga_{0.47}As$-InP quantum wells behave very similarly with those in the case of the GaAs-$Al_{0.3}Ga_{0.7}As$ quantum wells, while the former values are a little smaller than those of the latter.

These results can be applied to the analysis on the emission or absorption spectra in the heterosrtucture quantum wells, in which exciton binding and transition energies can be determined.

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