Internal transitions of confined magnetoexcitons in GaAs-(Ga,Al)As quantum wells

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Internal transitions of confined magnetoexcitons in GaAs-(Ga,Al)As quantum wells have been theoretically studied under magnetic fields applied along the growth direction. Results are obtained within the effective-mass approximation and by using a variational procedure. Calculations are performed for transitions from $1s$-like to $2p$-, $3p$-, and $4p$-like magnetoexciton states as functions of the applied magnetic field, and for several well widths. Theoretical results for the far-infrared intraexcitonic transition energies are then compared with recent experimental measurements using optically detected resonance techniques.

In the last two decades there has been considerable interest in the study of excitonic states[1–8] in low-dimensional semiconductor heterostructures. In particular, magneto-optical properties have been studied in both type-I and type-II semiconductor superlattices by means of absorption, photoluminescence, magnetoreflectance, and other techniques. Experimental results have shown that excitons have discrete internal energy levels, behaving essentially as ''atoms in semiconductors,'' and the transition energies of excitons in semiconductor superlattices are found in the far-infrared region.

Recently, Černe *et al.*[5] have investigated the terahertz (THz) dynamics of magnetoexcitons in GaAs-(Ga, Al) As undoped multiple quantum wells (MQW's) under magnetic fields applied perpendicular to the well interfaces, and observed resonant far-infrared (FIR) absorption by the confined magnetoexcitons. The dominant resonance in GaAs-$Ga_{0.7}Al_{0.3}$As MQW's (with well and barrier widths of 100 and 150 Å, respectively) was assigned to the $1s\rightarrow 2p_+$ intraexcitonic transition of the heavy-hole exciton. The absorption feature was found to persist even when the FIR electric field is comparable to the electric field that binds the exciton. Similar results were obtained by Salib *et al.*[6] and Nickel *et al.*[7,8] who performed a detailed optically detected resonance (ODR) experimental study of internal transitions of confined magnetoexcitons in two GaAs-$Ga_{0.7}Al_{0.3}$As MQW structures (125-Å well/150-Å barrier, and 80-Å well/150-Å barrier), with several resonances assigned to $1s\rightarrow 2p_+$, $3p_+$, and $4p_+$ internal excitonic transitions.

In this work we are concerned with a theoretical study, within the effective-mass approximation and following a variational procedure, of the properties of magnetoexcitons in GaAs-(Ga, Al) As QW's. In particular, we are interested in evaluating the internal magnetoexciton transitions in GaAs-$Ga_{0.7}Al_{0.3}$As QW's in order to compare with the experimental data by Cerne *et al.*,[5] Salib *et al.*,[6] and Nickel *et al.*[7,8]

We consider exciton states in a GaAs QW of width L surrounded by $Ga_{1-x}Al_x$As barriers in the presence of a magnetic field parallel to the growth direction. We work in the effective-mass approximation, and assume a parabolic dispersion for electrons and a four band model for holes, although, for simplicity, we discard the off-diagonal elements in the hole Hamiltonian, i.e., effects due to hole subband mixing are not included in the calculation. In addition, we have assumed the GaAs values for the conduction- and valence-band mass parameters in both GaAs and $Ga_{1-x}Al_x$As, and neglected effects due to the small difference in the dielectric constant of well and barrier materials, i.e., image-charge effects are not considered and the electron-hole Coulomb interaction is assumed to be screened by the GaAs static dielectric constant. The values of the potential-well barriers V_c and V_v are determined from the Al concentration and assumed to be 60 and 40% of the total energy-band-gap discontinuity, respectively.[1] Moreover, for an exciton confined in a semiconductor QW, we take the exciton envelope wave function as proportional to $(e^{i\vec{K}\cdot\vec{R}}/\sqrt{S})\psi_E(\vec{\rho},z_e,z_h)$, where S is the transversal area of the QW, $\vec{K}$ is the exciton in-plane wave vector, $\vec{\rho}$ is the xy relative coordinate, and $\vec{R}$ is the in-plane coordinate of the exciton center of mass. One may write

$$\psi_E(\vec{\rho},z_e,z_h)=f_e(z_e)f_h(z_h)\phi_E(\vec{\rho},z_e,z_h), \tag{1}$$

where f_e and f_h are the z part of the QW electron and hole wave functions,[1] respectively, in the absence of the Coulomb potential, and assume that the relative motion of carriers and of the center of mass are independent. The heavy-hole ($J_z^h = \pm\frac{3}{2}$) and light-hole ($J_z^h = \pm\frac{1}{2}$) exciton Hamiltonians, with energies—measured with respect to the band gap of the GaAs bulk material—expressed in units of rydbergs ($R_0 = m_0 e^4/2\hbar^2$), lengths in hydrogen Bohr radii ($a_0 = \hbar^2/m_0 e^2$), and magnetic fields in terms of the dimensionless quantity $\gamma = e\hbar B/2m_0 c R_0$, may be taken as[3,9]

$$H^{\mathrm{exc}}_{\pm 3/2} = -\frac{m_0}{m_e}\frac{\partial^2}{\partial z_e^2} + V_c(z_e) - \frac{1}{m_h^{\pm 3/2}}\frac{\partial^2}{\partial z_h^2} + V_v(z_h) + (\gamma_1 + \gamma_2 + m_0/m_e)\left(-\nabla^2_{\vec{\rho}} + \frac{\gamma^2\rho^2}{4}\right) + (-\gamma_1 - \gamma_2 + m_0/m_e)\gamma L_z \pm \left(3\kappa + \frac{27}{4}q\right)\gamma - \frac{2}{\varepsilon|\mathbf{r}_e - \mathbf{r}_h|} \pm \frac{g_e}{2}\gamma, \tag{2}$$

$$H^{\mathrm{exc}}_{\pm 1/2} = -\frac{m_0}{m_e}\frac{\partial^2}{\partial z_e^2} + V_c(z_e) - \frac{1}{m_h^{\pm 1/2}}\frac{\partial^2}{\partial z_h^2} + V_v(z_h) + (\gamma_1 - \gamma_2 + m_0/m_e)\left(-\nabla^2_{\vec{\rho}} + \frac{\gamma^2\rho^2}{4}\right) + (-\gamma_1 + \gamma_2 + m_0/m_e)\gamma L_z \pm \left(\kappa + \frac{1}{4}q\right)\gamma - \frac{2}{\varepsilon|\mathbf{r}_e - \mathbf{r}_h|} \pm \frac{g_e}{2}\gamma, \tag{3}$$

with

$$L_z = \frac{\partial}{i\,\partial\phi} \tag{4}$$

as the operator for the orbital angular momentum in the z direction, and

$$\nabla^2_{\vec{\rho}} = \frac{\partial^2}{\partial\rho^2} + \frac{1}{\rho}\frac{\partial}{\partial\rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial\phi^2} \tag{5}$$

is the two-dimensional Laplacian in the QW plane. The GaAs conduction-band effective mass is taken as $m_e = 0.067 m_0$ (where m_0 is the free-electron mass),

$$1/m_h^{\pm 3/2} = \gamma_1 - 2\gamma_2, \tag{6}$$

$$1/m_h^{\pm 1/2} = \gamma_1 + 2\gamma_2, \tag{7}$$

the Luttinger[9] valence-band parameters[1,3] are taken as $\gamma_1 = 7.36$, $\gamma_2 = 2.57$, $\kappa = 1.2$, $q = 0.04$, and the g factor of the conduction-band electron[3] as $g_e = -0.44$. For simplicity, we consider orthogonalized[10] variational wave functions, i.e., we take

$$\phi_E(\vec{\rho}, z_e, z_h) = \rho^{|m|}\exp(im\phi)P_{n,l}(r)\exp(-\lambda_{n,l} r) \tag{8}$$

in Eq. (1), where the $P_{n,l}(r)$, with $r = \sqrt{\rho^2 + (z_e - z_h)^2}$, are hydrogeniclike polynomial functions for exciton states with principal quantum number n and orbital quantum number l, and the $\lambda_{n,l}$ are variational parameters. In what follows, magnetoexciton energy states are labeled as $nlm(J_z^e, J_z^h)$

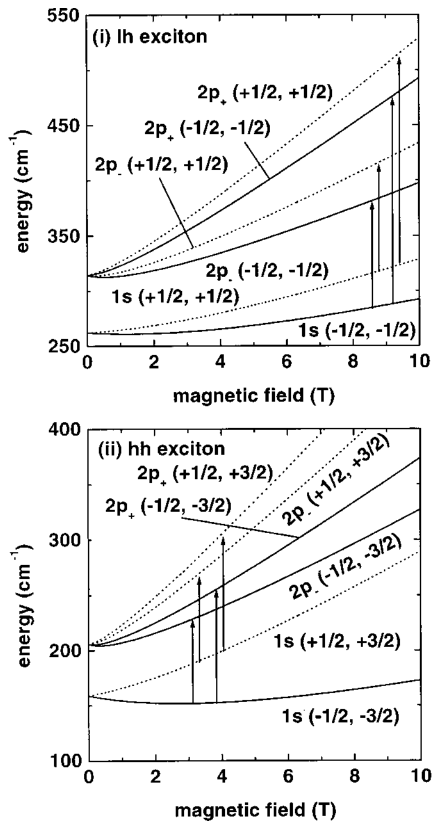

FIG. 1. Calculated variational energies of the $1s$ and $2p_\pm$ states of the light-hole (i) and heavy-hole (ii) magnetoexcitons as functions of the growth-direction applied magnetic field for an $L = 125$-Å GaAs-$Ga_{0.70}Al_{0.30}As$ QW. Magnetoexciton energy states are labeled as $n\ell m(J_z^e, J_z^h)$ which correspond to an $n\ell m$-like exciton state composed of a J_z^e electron (with $J_z^e = \pm\frac{1}{2}$) and a J_z^h hole (with $J_z^h = \pm\frac{1}{2}, \pm\frac{3}{2}$). Vertical arrows indicate spin-conserving magnetoexciton $1s \rightarrow 2p_\pm$ transition energies.

which correspond to an *nlm*-like exciton state composed of a J_z^e electron (with $J_z^e = \pm\frac{1}{2}$) and a J_z^h hole (with $J_z^e = \pm\frac{1}{2}, \pm\frac{3}{2}$).

We have performed variational calculations for heavy- ($J_z^h = \pm\frac{3}{2}$) and light-hole ($J_z^h = \pm\frac{1}{2}$) magnetoexciton states in GaAs-$Ga_{0.7}Al_{0.3}As$ QW's and compare theoretical results with recent intraexcitonic experimental data obtained via optically detected resonant techniques.[5–8] One should note that actual measurements are for GaAs-$Ga_{0.7}Al_{0.3}As$ superlattices and, for simplicity, we have ignored tunneling effects and performed calculations for single *isolated* GaAs-$Ga_{0.7}Al_{0.3}As$ QW's.

The growth-direction magnetic-field dependence of the $1s$ and $2p_\pm$ light- and heavy-hole magnetoexciton variational energies are displayed in Fig. 1, in the case of an $L = 125$-Å GaAs-$Ga_{0.70}Al_{0.30}As$ QW. There, we also indicate (see arrows in Fig. 1) possible spin-conserving $1s \rightarrow 2p_\pm$ intraexcitonic transition energies. In that respect, if one looks at the light-hole spin-conserving intraexcitonic transitions such as $1s\ (-\frac{1}{2}, -\frac{1}{2}) \rightarrow 2p_-\ (-\frac{1}{2}, -\frac{1}{2})$ or $1s\ (+\frac{1}{2}, +\frac{1}{2}) \rightarrow 2p_-\ (+\frac{1}{2}, +\frac{1}{2})$, for example, both transitions have the same energy, as one would expect from the spin-dependence of the Hamiltonian [cf. Eqs. (2) and (3)]. Although not shown in Fig. 1, we have also performed calculations for the $3p_\pm$ light- and heavy-hole magnetoexciton states in an L

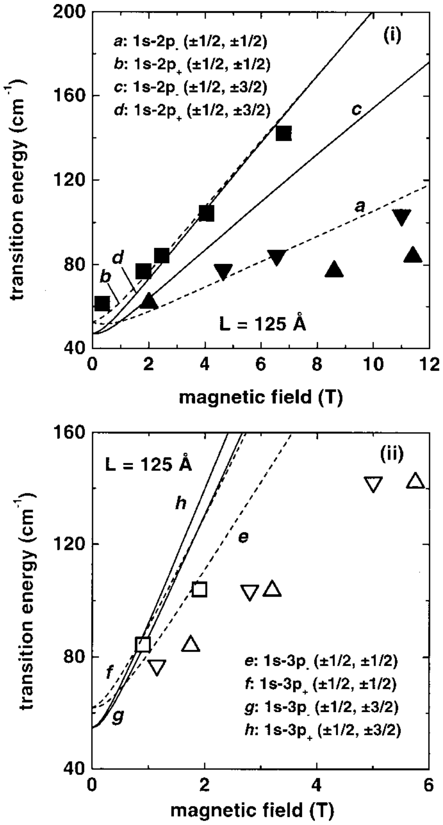

FIG. 2. Light-hole (dashed curves) and heavy-hole (full curves) spin-conserving $1s \rightarrow 2p_{\pm}$ (i) and $1s \rightarrow 3p_{\pm}$ (ii) theoretical magnetoexciton transition energies in an $L=125$-Å GaAs-$Ga_{0.70}Al_{0.30}$As QW as functions of the growth-direction applied magnetic field. Also shown are the experimental results of Nickel *et al.* (Refs. 7 and 8).

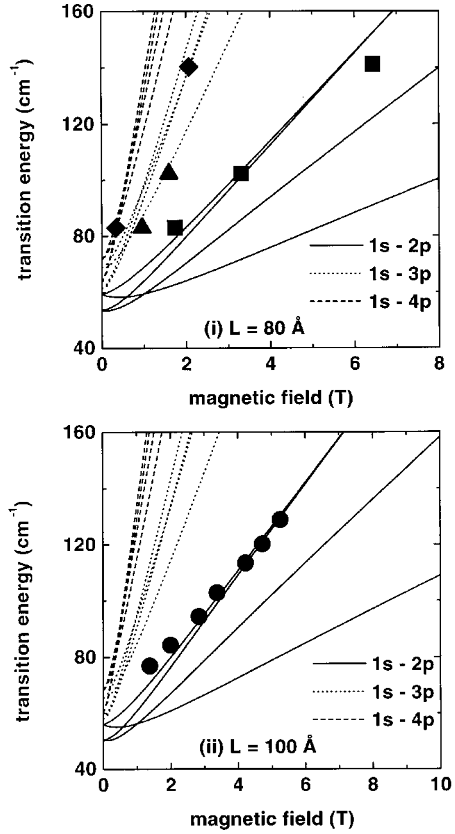

FIG. 3. Light-hole and heavy-hole spin-conserving $1s \rightarrow np_{\pm}$ ($n=2,3,4$) theoretical magnetoexciton transition energies in $L=80$ Å and $L=100$ Å (ii) GaAs-$Ga_{0.70}Al_{0.30}$As QW's as functions of the growth-direction applied magnetic field. Also shown are the experimental results of Salib et al. (Ref. 6) and Černe *et al.* (Ref. 5).

$=125$-Å GaAs-$Ga_{0.70}Al_{0.30}$As QW. The magnetic-field dependence of the spin-conserving intramagnetoexciton light- and heavy-hole $1s \rightarrow 2p_{\pm}$ and $1s \rightarrow 3p_{\pm}$ transition energies are shown in Fig. 2 for an $L=125$-Å GaAs-$Ga_{0.70}Al_{0.30}$As QW and compared with the experimental results by Nickel *et al.*[7,8] As can be seen from Fig. 2 (i), the variational theoretical results for the $1s \rightarrow 2p_{+}$ intraexcitonic light- ($J_z^h = \pm\frac{1}{2}$) and heavy-hole ($J_z^h = \pm\frac{3}{2}$) transitions (curves *b* and *d*, respectively) are in quite good agreement with the experimental data (set of full squares) by Nickel *et al.*,[7,8] and suggest that these observed intraexcitonic transitions occur in both heavy- and light-hole magnetoexcitons. This contrasts with the assignment by Salib *et al.*[6] and Nickel *et al.*[7,8] of the observed (see set of full squares) intraexcitonic transitions to nearly degenerate $1s \rightarrow 2p_{+}$ heavy-hole transitions. Also, theoretical $1s \rightarrow 2p_{-}$ intraexcitonic light- ($J_z^h = \pm\frac{1}{2}$) and heavy-hole ($J_z^h = \pm\frac{3}{2}$) transitions (curves *a* and *c*, respectively) reproduce the qualitative features of the magnetic-field dependence of the experimental data by Nickel *et al.*[7,8] [see full up and down triangles in Fig. 2 (i)], although quantitative agreement is clearly not good. Theoretical curves and open experimental[7,8] symbols in Fig. 2 (ii) correspond to $1s \rightarrow 3p_{\pm}$ light- and heavy-hole intraexcitonic transition energies, and again only qualitative features are loosely reproduced.

Theoretical results for the $1s \rightarrow 2p$, $1s \rightarrow 3p$, and $1s \rightarrow 4p$ light- and heavy-hole intraexcitonic transition energies for $L=80$- and 100-Å GaAs-$Ga_{0.70}Al_{0.30}$As QW's are displayed in Fig. 3 in comparison with experimental measurements by Salib *et al.*[6] and Černe *et al.*,[5] respectively. Variational theoretical results for the $1s \rightarrow 2p_{+}$ intraexcitonic light- ($J_z^h = \pm\frac{1}{2}$) and heavy-hole ($J_z^h = \pm\frac{3}{2}$) transitions are in excellent agreement with the experimental data for both $L=80$- and 100-Å GaAs-$Ga_{0.70}Al_{0.30}$As QW's. The two up-triangle experimental transitions by Salib *et al.*[6] are in good agreement with the theoretical $1s \rightarrow 3p_{-}$ light-hole ($J_z^h = \pm\frac{1}{2}$) intraexcitonic transitions. On the other hand, the assignment of the two full diamond experimental features to specific intraexcitonic transitions is uncertain, in our opinion, and would certainly require further experimental and theoretical work.

To conclude, we have made a systematic study of $1s \rightarrow 2p_{\pm}$, $1s \rightarrow 3p_{\pm}$, and $1s \rightarrow 4p_{\pm}$ light- and heavy-hole magnetoexcitonic transition energies in GaAs-$Ga_{1-x}Al_x$As QW's within a variational procedure in the effective-mass approximation. Although some of the theoretical magnetoexciton transition energies agree very well with experimental measurements, other calculated results only reproduce qualitative features and quantitative agreement is not good. We believe that effects due to hole subband mixing, which are not included in the present work, should be taken into account for a proper quantitative understanding of the experimental data. Also, several theoretically possible magnetoexciton transitions do not show up in the experimental spectra and, in this respect, a theoretical calculation of the intraexcitonic absorption line shape, as well as further experimental and theoretical work, would certainly be of considerable importance for a better understanding to be achieved.

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