Magnetic Field Effects in the Optical Absorption of Shallow Donor Impurities in Quantum Wells

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We present a. calculation of tlie optical absorption for different intraimpurity transitions inside a $Ga_{1-x}Al_xAs/GaAs$ quantum well under strong magnetic field. In the dilute regime t ıe effects of compensation and well width are taken into account in the calculation by a Monte Carlo simulation of the position of impurities. Results for $1s \rightarrow 2p_+$ transition energy are in good agreement with effective mass calculations and experimental values available in tlie literature.

In tliis work we present an investigation of the infrared absorption coefficient of shallow donor impurities inside a $Ga_{1-x}Al_xAs/GaAs$ quantum well (QW) under a strong magnetic field. Our model is based on a recent analysis of line broadening for absorption[1,2] as well as recent measurement on far-infrared magnetospectroscopy of impurities at tlie center of $GaAs$ quantum wel s[3]. The absorption coefficient is obtained through a Monte Carlo simulation[2,4]. Results for 1s $\rightarrow$ $2p_+$ transition energy when compared to other calculations[5] and experimental data[3] show a very good agreement between them.

Tlie Hamiltonian of an electron bound to a shallow donos placed inside a QW, when a uniform magnetic field B is applied perpendicular to its interfaces is written as[2]:

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + \frac{e^2B^2}{8m^*c^2}\rho^2 - \frac{eB}{2m^*c}L_z - \frac{e^2}{Ku} + V(z), \quad (1)$$

with L, being the z-component of the angular momentum operator and ρ tlie radial distance from the z-axis, m* be the effective mass of the electron, K the effective dielectric constant of the QW, e the electronic charge and u the clistance between the electron and the donor.

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$V(z)$ is tlie confining potential described, in the model of infinite barriers, as:

$$V(z) = \begin{cases} 0 & \text{if } |z| < \frac{L}{2} \\ \infty & \text{if } |z| > \frac{L}{2} \end{cases} \quad (2)$$

where L is tlie width of tlic QW. The effective units used are:

$$a^* = \frac{\hbar^2 K}{m^* e^2}\,, \quad (3)$$

tlie effective Bohr radius (in GaAs **1** $a^* \approx 100\mathring{A}$) and

$$Ry^* = \frac{m^* e^4}{2\hbar^2 K^2}\,, \quad (4)$$

the effective rydberg (in GaAs **1** $Ry^* \approx 5.8$meV). Expressing tlie magnetic field in terms of the cyclotron frequency

$$\omega_c = \frac{-eB}{m^* c}, \quad (5)$$

we have

$$H = -\nabla^2 - \frac{2}{u} + \frac{1}{2}\frac{\gamma}{\hbar}L_z + \frac{1}{16}\gamma^2\rho^2 + V(z), \quad (6)$$

where γ is defined as

$$\gamma = \frac{\hbar\omega_c}{Ry^*}\,, \quad (7)$$

(for GaAs we have $B = 3.3\gamma$ tesla). We write the wave functions as:

$$\Psi_{ns}(\mathbf{r}) = \Phi_{SB}(z)P_{n-1}(u)e^{-(\kappa_{ns}u+\eta_{ns}\rho^2)}\,, \quad (8)$$

$$\Psi_{np\pm}(\mathbf{r}) = \Phi_{SB}(z)P_{n-2}(u)e^{-(\kappa_{np}u+\eta_{np}\rho^2)}\rho e^{\pm i\varphi}\,, \quad (9)$$

where

$$\Phi_{SB}(z) = \cos\left(\frac{\pi z}{L}\right) \quad (10)$$

is the ground state wave function of the QW, κ's and η's are the variational parameters and $P_n(u)$ is a n-degree polynomial.

The energies of tlie compensated system and of an electron bound to the k-th donor are, respectively

$$E_S = \frac{e^2}{K}\left[\frac{1}{2}\sum_{\substack{k\neq l \\ (don)}}\frac{(1-n_l)(1-n_k)}{r_{kl}} - \sum_{\substack{k \\ (don)}}\sum_{\substack{i \\ (acc)}}\frac{1-n_k}{r_{kj}} + \frac{1}{2}\sum_{\substack{i\neq j \\ (acc)}}\frac{1}{r_{ij}}\right] + \sum_{\substack{k \\ (don)}} n_k \quad \epsilon_k^{(0)} \quad (11)$$

and

$$\epsilon_k = \frac{e^2}{K}\left[\sum_{\substack{j \\ (acc)}}\frac{1}{r_{kj}} - \sum_{\substack{l(\neq k) \\ (don)}}\frac{1-n_l}{r_{kl}}\right] + \epsilon_k^{(0)}\,. \quad (12)$$

Here $\{n_k\}$ is the set of donor occupation numbers determining the ground state, r_{ij} is tlie distance between the i-th and j-th impurities and $\epsilon_k^{(0)}$ is the energy of an electron bound to a donor without the electrostatic contribution of the ionized impurities. The terms (don) and (acc) mean donor and acceptor respectively. The positions of impurities and $\{n_k\}$ are generated by Monte Carlo simulation.

The absorption coefficient due to the k-th electron

is then obtained by the relation

$$\hbar\omega W(z_k,\omega) = \sigma_1(z_k,\omega)\langle\mathcal{E}^2\rangle \ , \qquad (13)$$

where $\mathcal{E}$ is the electric field of the radiation

In the long wavelength approximation

$$\sigma_1(z_k,\omega) = \pi e^2\omega|\mathbf{u}\cdot\langle n|\mathbf{r}|m\rangle_k|^2\delta(E_{nm}(z_k)-\hbar\omega) \quad (14)$$

where $\mathbf{u}$ is the radiation's polarization and $\langle n|\mathbf{r}|m\rangle_k$ is the matrix element of the operator $\mathbf{r}$, taken between the states n and m of the k-th bound electron.

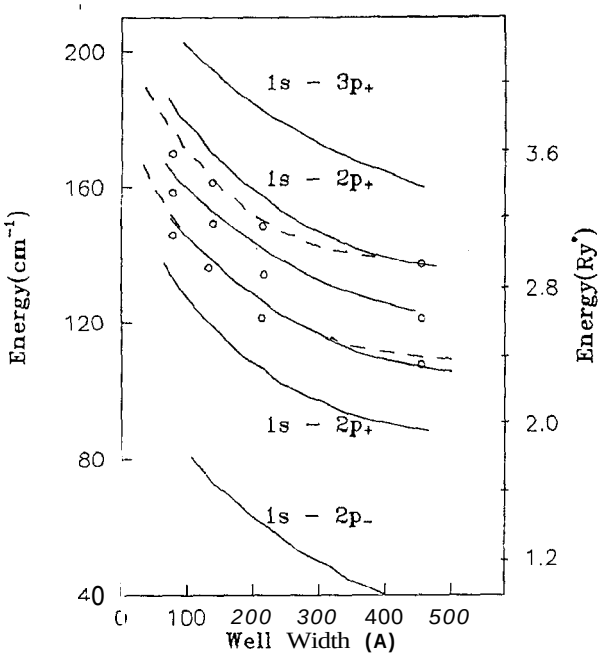

Figure 1: Energy of tlie $1s - 3p_+$, $1s \rightarrow 2p_+$ and $1.5 \rightarrow 2p_-$ transitions a:; a function of well width for various inagiietic fields. Open circles are experimental results for $1s \rightarrow 2p_+$ transition with $B = 5.0$, 6.0, aiid 7.0 T in descending order[3]. Broken liiies are tlie results for potential barrier of **0.323** eV [5] with $B = 7.03$ aiid 5.25 T respectively in descending order. Solid liiies are the results of our calculations. Tlie transition $1s - 3p_+$ corresponds to $B = 7.0$ T. In descending order to $1s \rightarrow 2p_+$, tlie magnetic fields correspond to $13 = 7.0$. 6.0, 5.0 and **3.3** T respectively. Tl e $1s \rightarrow 2p_-$ energy transitions corresponding to $B = 5.0$, 6 0 and 7.0 T present almost the same resuts. They are superimposed.

$W(z_k,\omega)$ is the transition rate per unit time for a donor electron localized at z_k, given by

$$W(z_k,\omega) = \frac{2\pi}{\hbar}|\langle n|\frac{-e}{m^*c}\mathbf{A}_{rad}\cdot\mathbf{P}|m\rangle|^2\delta(E_{nm}(z_k)-\hbar\omega) \qquad (15)$$

where m and n are the initial and final states respectively, $E_{nm}(z_k)$ is the difference in energy between the two electronic states and ω is the angular frequency of the radiation. 111 tlie dilute regime the average distance between impurities is much bigger than the effective Bohr radius and then we neglect overlap between states belonging to different donors. For that reason the absorption occurs intra-site and m and n refer to states belonging to the same impurity.

Oiicc we have tlie absorption coefficient for a single impurity, we can calculate it for the total number of impurities for a given configuration.

Tlie absorption coefficient of this system is obtained by an average over N configurations. Then

$$\sigma_1(\omega) = <\sigma_1(\omega)>_{config.} \qquad (16)$$

$$= \frac{1}{N}\sum_{\alpha=1}^{N}\sigma_1^{(\alpha)}(\omega) \ . \qquad (17)$$

In Fig. 1 we show the observed and calculated $1s \rightarrow 2p_+$ transition energy as well as $1s \rightarrow 2p_-$ and $1s \rightarrow 3p_+$ transitions. They are presented in QW's of different magnetic fields, for an impurity located on-center, as a. function of well width. We may note that the energies of the transition $1s \rightarrow 2p_-$ do not show an appreciable difference with the applied magnetic field. We can also see this effect in Fig. 3b.

In Fig. 2 we show tlie effect of well width L (with compensation 0.1 and magnetic fielcl of 3.3 T), on the

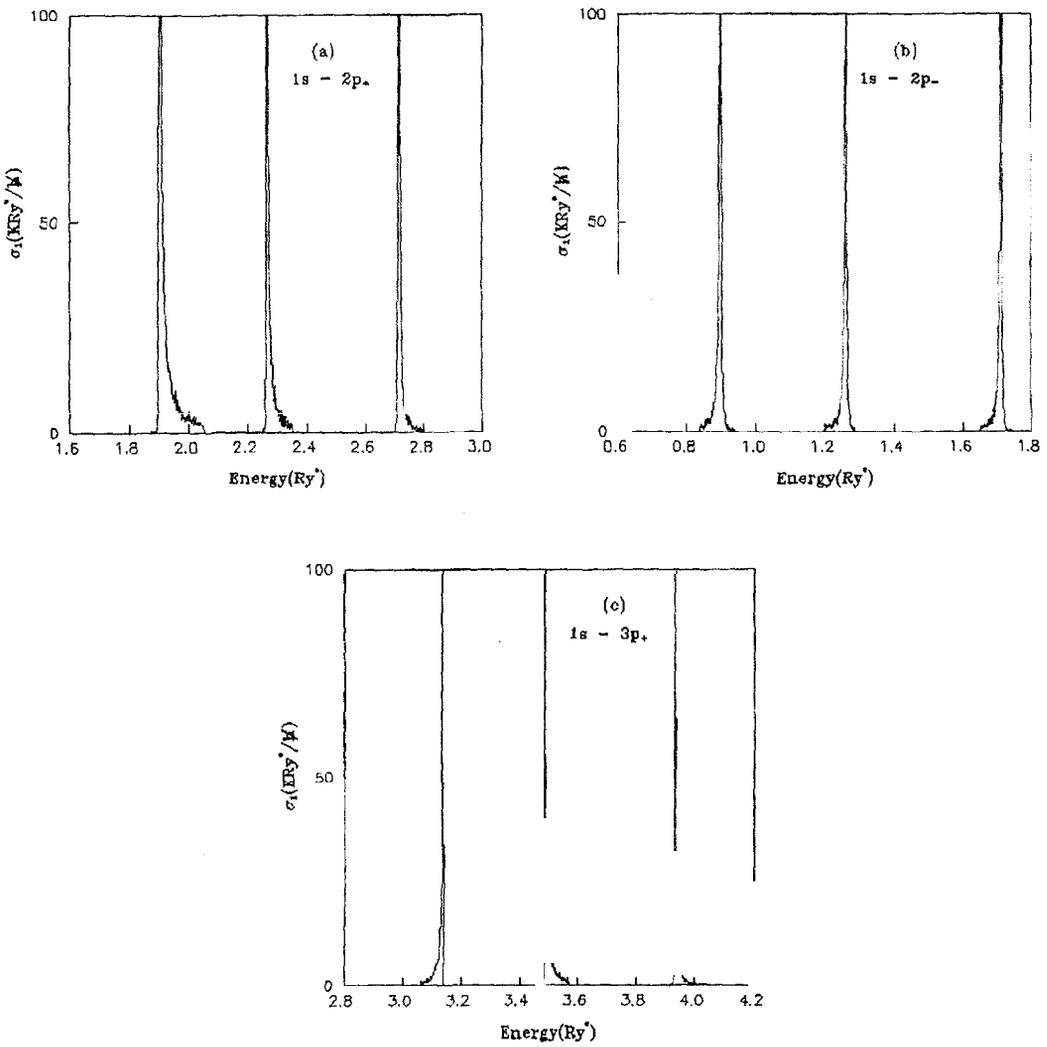

Figure 2: The effect of well width (in tlie order L = 400, 200 and 100 $\AA$ left to right) on the absorptioii coefficient for delta-doping profile at tlie centcr of tlie QW, with $B = 3.3T$ and compensation 0.1, of tlie transitions: (a)$1s \rightarrow 2p_+$, (b)$1s \rightarrow 2p_-$, and (c)$1s \rightarrow 3p_+$.

absorption coefficient for the transitions 1s $\rightarrow 2p_+$, $1s \rightarrow 2p_-$ and $1s \rightarrow 3p_+$. The increasing of the well width causes a shift in the absorption spectrum to lower energies.

In Fig. 3 we show tlie effect of magnetic field (1.65, 3.3 and 6.6 T, with L = 100$\AA$ and compensation 0.1) on the absorption coefficient for tlie above intraimpurity transitions. Increasing tlie magnetic field the absorption spectrum is shifted to higher energies. This effect does not occur in the transition $1s \rightarrow 2p_-$ because the linear term in γ in equation 6, foi low magnetic field, is predominant over the quadratic term.

We note in figures 2a, 2b, 3a and 3b a similar inhomogeneity as observed by Larsen[7] in bulk materials. All the calculations are performed for on-center delta-doping with impurity concentration of 1.0 x $10^{10} cm^{-2}$.

Briefly, we have investigated different intraimpurity transition energies, which show for $1s \rightarrow 2p_+$ a very good agreement with experimental data[3,6]. A Monte Carlo simulation was used to take into accoiint a distribution of impurities, producing an asymmetric line broadening of the absorption spectra for different transitions, magnetic fields and well widths.

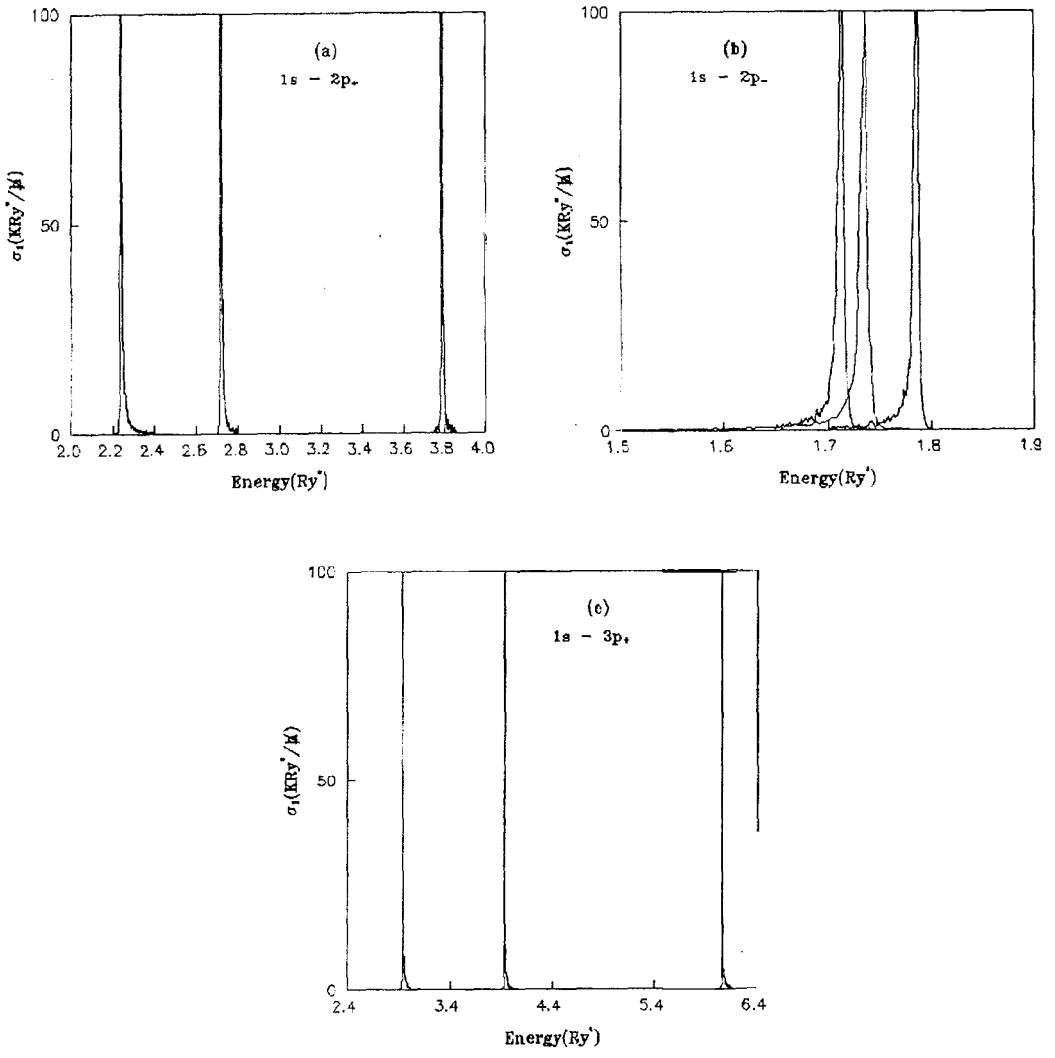

Figure 3: The effect of magnetic field on tlie absorption coefficient for delta-doping profile at the center of tlie QW, with $L = 100$ Å and compensation 0.1 of tlie transitions: (a) $1s \rightarrow 2p_+$, (c) $1s - 3p_+$ (botli in tlie order B = 1.65, **3.3** and 6.6 T left. to right) and (b) $1s - 2p_-$ (in the order B = 3.3, 1.65 and 6.6 T).

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