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Donor-related magneto-optical absorption spectra of GaAs–(Ga, Al)As quantum wells

L H M Barbosa†, A Latgé†, L E Oliveira‡ and M de Dios-Leyva§

† Instituto de Física, Universidade Federal Fluminense, 24210-340, Niterói-RJ, Brazil
‡ Instituto de Física, CP 6165, Unicamp, Campinas, São Paulo, 13083-970, Brazil
§ Department of Theoretical Physics, University of Havana, San Lazaro y L, Vedado, 10400, Havana, Cuba

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Abstract. The effects of applied magnetic fields on the optical absorption spectra associated with transitions from the Landau valence magnetic levels to shallow donor states in GaAs–(Ga, Al)As quantum wells are studied for magnetic fields applied perpendicular to the heterostructure interfaces. The donor-related magneto-absorption spectra are calculated within the effective-mass approximation, and with a minimization procedure for evaluating donor energies and envelope wave functions. We consider a homogeneous donor distribution in the well and analyse the theoretical impurity-related magneto-absorption spectra for various quantum well widths and applied magnetic fields. The magneto-absorption lineshapes present features clearly associated with transitions involving donor states and different valence Landau magnetic levels.

1. Introduction

Due to the potential device applications of doped semiconducting superlattices and heterostructures, there has been a considerable interest in the physical properties associated with these systems. The understanding of the nature of impurity states associated with heterostructures is a subject of considerable technical and scientific relevance. The optical absorption spectra associated with transitions involving shallow impurities in quantum wells (QWs) was studied by Bastard [1], who considered an infinite-barrier QW and studied the hydrogenic-impurity states within a variational procedure. His work was followed by a more detailed investigation by Oliveira and co-workers [2] who analysed the absorption and photoluminescence spectra associated with shallow donors and acceptors in GaAs–(Ga, Al)As QWs. Experimentally, the observation of acceptor-related features in the photoluminescence spectra of GaAs–(Ga, Al)As QWs and superlattices was reported by Miller *et al* [3], and properties of donors in those systems have been studied by Shanabrook and co-workers [4] and Helm *et al* [5].

Concerning the magneto-optical properties of semiconducting heterostructures, experimental techniques such as interband magnetoluminescence and cyclotron resonance [6, 7] have been used to study the effects of applied magnetic fields in superlattices in both configurations, parallel and perpendicular to the interfaces. Belle *et al* [8] have shown, both theoretically and experimentally, that transitions between well-defined Landau levels may be seen in the interband magnetoluminescence only for transitions that are related to Landau levels with energies within the first electron and hole minibands. de Dios-Leyva and Galindo [9] calculated the absorption coefficient of GaAs–(Ga, Al)As superlattices under an in-plane magnetic field for the case of intraband transitions between electronic magnetic levels. The observation of an intersubband donor-absorption line induced by applying an in-plane magnetic field in a QW was reported by Brozak *et al* [10]. Via photoluminescence measurements associated with transitions from the conduction band to acceptor states in applied magnetic fields, Skromme *et al* [11] have investigated the cyclotron motion of electrons in multiple QW. Although there has been quite a considerable amount of experimental and theoretical work on hydrogenic impurities in QWs and superlattices, there are still some theoretical and experimental aspects to be considered on impurity-related absorption in QWs.

In this work we present a systematic study of the magneto-optical absorption spectra associated with donors in GaAs–(Ga, Al)As QWs under magnetic fields applied in the QW growth direction, and consider transitions between the valence Landau states and ground-state donor levels. The temperature is assumed high enough ($T \gg 100$ K) that each donor state is ionized. Section 2 will be devoted to the presentation of some theoretical aspects and to the calculation of the transition probability per unit of time associated with the donor-related magneto-optical absorption spectra. Results and a discussion are presented in section 3 and our conclusions are in section 4.

2. Theory

In the effective-mass approximation, the Hamiltonian for a donor impurity in a GaAs–(Ga, Al)As QW, under a magnetic field $\boldsymbol{B}$ applied perpendicular to the interfaces, may be written as

$$H = \frac{1}{2m^*}\left(\boldsymbol{p} + e\frac{\boldsymbol{A}}{c}\right)^2 - \frac{e^2}{\epsilon r} + V_b(z) \tag{1}$$

where, $\boldsymbol{A} = \boldsymbol{B} \times \boldsymbol{r}/2$ is the magnetic vector potential, $r = [\rho^2 + (z - z_i)^2]^{1/2}$, z_i is the position of the impurity with respect to the $z = 0$ origin chosen at the centre of the well, $\epsilon = 13.1$ is the dielectric constant [12], m^* is the conduction-band effective mass ($m^* = m_c^* = 0.0665\ m_0$; m_0 is the free-electron mass), and we assume the values of m^* and ϵ for GaAs for all regions of the heterostructure. The barrier potential $V_b(z)$ is taken as a square well of width L and height V_b. The size V_b of the barrier is taken to be 60% of the band-gap discontinuity ΔE_g (eV) $= 1.247x$ in the GaAs–$Ga_{1-x}Al_xAs$ heterostructure for the conduction band [3, 13]. For the valence-band states, we neglect the effect of coupling of the top four valence bands [14] of both well and barrier semiconductors and consider a spherical-carrier effective mass $m_v^* \simeq 0.3\ m_0$ which gives an experimental bulk value [3, 15] of 26 meV for the acceptor binding energies. We follow a minimization procedure for evaluating donor energies and envelope wave functions, which are taken as products of the QW ground-state solution and the variational hydrogenic 1s-like functions [16].

The donor-related magneto-optical absorption is associated with transitions involving valence Landau magnetic levels and donor states. The envelope wave function of the $|i\rangle$ initial (valence) state is taken as

$$F_i = \frac{e^{im\phi}}{\sqrt{2\pi}} f_v(z) U_{n_r m}(\rho) \tag{2}$$

where

$$U_{n_r m}(\rho) = \sqrt{\frac{n_r!}{(n_r + |m|)!\, l_H^2}} \left(\frac{\rho}{\sqrt{2} l_H}\right)^{|m|} \exp\left(-\frac{\rho^2}{4 l_H^2}\right) L_{n_r}^{|m|}\left(\frac{\rho^2}{2 l_H^2}\right) \tag{3}$$

where $L_{n_r}^{|m|}$ is the associated Laguerre polynomial, n_r and m are quantum numbers, and $l_H = \sqrt{\hbar c/eB}$ is the usual Landau length. For the envelope wave function of the $|f\rangle$ final donor state, we used the trial wave function

$$F_f = N_c f_c(z) \mathrm{e}^{-\{\alpha r + \beta\rho^2 + \gamma(z-z_i)^2\}} \tag{4}$$

where α, β, and γ are variational parameters [17], and N_c is a normalization factor. In equations (2) and (4), f_c and f_v are the z-solutions of the conduction and valence envelope wave functions for the QW in the absence of the magnetic field. The above variational wave function gives good agreement with experiment as demonstrated in recent theoretical work [16, 18].

Taking the origin at the bottom of the conduction band, we have for the initial and final energies

$$E_i = -E_g - E_{1v} - \hbar\omega_v\left(n_r + \frac{|m| + m}{2} + \frac{1}{2}\right) \tag{5}$$

and

$$E_f = E_{1c} + \frac{1}{2}\hbar\omega_c - E(L, z_i) \tag{6}$$

where $\omega_{c,v} = eB/cm^*_{c,v}$ are the conduction (valence) cyclotron frequencies, $E(L, z_i)$ is the donor binding energy, E_g is the bulk GaAs gap, and $E_{1c(1v)}$ is the bottom (top) of the first conduction (valence) subband.

The transition rate associated with transitions from the valence Landau levels to 1s-like donor states is calculated using the Fermi golden rule:

$$W(w) = \frac{2\pi}{\hbar}\sum_i |\langle f|H_{int}|i\rangle|^2 \delta(E_f - E_i - \hbar\omega) \tag{7}$$

with

$$H_{int} = \frac{e}{m_0 c}\boldsymbol{A}_{ph}\cdot\left(\boldsymbol{p} + \frac{e}{c}\boldsymbol{A}\right)$$

where $\boldsymbol{A}_{ph}$ is the radiation-field vector potential. The above matrix element may be written as [19]

$$\langle f|H_{int}|i\rangle = \frac{e}{m_0 c}\boldsymbol{A}_{ph}\cdot\boldsymbol{P}_{fi} S_{fi} \tag{8}$$

with

$$\boldsymbol{P}_{fi} = \frac{1}{\Omega_0}\int_{\Omega_0} \mathrm{d}\boldsymbol{r}\ u_f^*(\boldsymbol{r})\boldsymbol{p}\, u_i(\boldsymbol{r}) \tag{9}$$

and

$$S_{fi} = \int \mathrm{d}\boldsymbol{r}\ F_f^*(\boldsymbol{r}) F_i(\boldsymbol{r}) \tag{10}$$

where Ω_0 denotes the volume of the crystal unit cell, and u_f (u_i) is the periodic part of the Bloch function for the final (initial) state.

For a GaAs–$Ga_{1-x}Al_xAs$ QW of width L, the transition rate for valence-to-donor transitions (associated with a single impurity located at $z = z_i$) is therefore given by

$$\begin{aligned} W(w) = \frac{(2\pi)^2}{\hbar^2}\left(\frac{e}{m_0 c}\right)^2 |\boldsymbol{A}_{ph}\cdot\boldsymbol{P}_{fi}|^2 N_c^2 \left(\frac{1}{l_H}\right)^2 \\ \times \sum_{n_r}\sum_{z_i}\left|\int_{-\infty}^{\infty} \mathrm{d}z\ f_c(z) f_v(z)\exp\{-\gamma(z-z_i)^2\} I_{n_r}(z-z_i)\right|^2 \\ \times\ \delta(E_f - E_i - \hbar\omega) \end{aligned} \tag{11}$$

where

$$I_{n_r}(z - z_i) = \frac{e^{b(z-z_i)^2} e^{\alpha/(2\sqrt{b})}}{b} J_{n_r}(z - z_i) \tag{12}$$

where $b = \beta + 1/(4l_H^2)$, and J_{n_r} is an integral involving exponential functions (see equations (3) and (4)) and Laguerre polynomials. In obtaining the above transition rate, we have used the $m = 0$ selection rule which is the appropriate one for transitions from valence states to shallow donor 1s states.

We consider a homogeneous donor distribution inside the QW and assume that the quantum well thickness is much larger than the lattice spacing, so that the sum over impurity positions in equation (11) may be evaluated by means of an integral with respect to z_i across the whole well width. In order to introduce scattering effects, we replace the delta function with a Lorentzian with a width equal [20] to 0.50 meV.

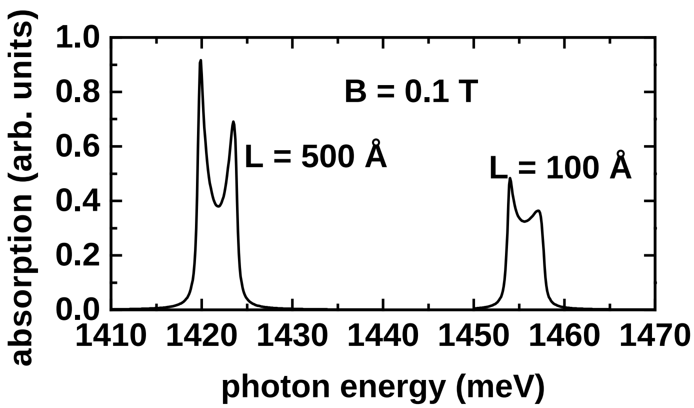

Figure 1. Magneto-optical absorption spectra associated with transitions from valence Landau levels to donor states, under $B = 0.1$ T, of GaAs–$Ga_{0.7}Al_{0.3}As$ QWs of widths $L = 100$ Å and $L = 500$ Å.

3. Results and discussion

The donor-related magneto-absorption spectra (equation (11)) are calculated for GaAs–$Ga_{0.7}Al_{0.3}As$ QWs, and for various well widths and applied magnetic fields. Figure 1 presents the calculated results for the magneto-absorption spectra related to transitions from the first valence Landau level to donor states for $L = 100$ Å and $L = 500$ Å QWs under a small magnetic field of 0.1 T (applied perpendicular to the interfaces). A considerable shift of the magneto-absorption spectra to smaller photon energies as the well width increases is apparent, as expected. Also, these results for small magnetic fields are in agreement with previous theoretical calculations by Oliveira and Pérez-Alvarez [2] for QWs in the absence of a magnetic field, in which one finds structures in the absorption spectra associated with on-centre and on-edge donors. The effects of an applied magnetic field of 5 T on the donor-related magneto-absorption spectra of GaAs–$Ga_{0.7}Al_{0.3}As$ QWs are shown in figure 2, in which we consider transitions involving three valence Landau magnetic levels, $n = n_r = 0, 1$, and 2, and 1s-like donor states. One notices that the total magneto-absorption spectra present features related to transitions associated with the three above-mentioned Landau levels. It is easy to verify that the separation between peaks is

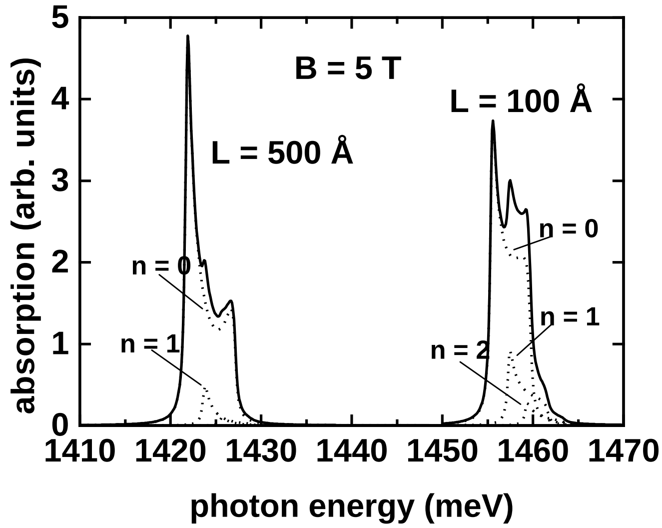

Figure 2. Magneto-optical absorption spectra associated with transitions from $n = 0$, 1, and 2 valence Landau levels (dotted lines) to donor states, under $B = 5$ T, of GaAs–$Ga_{0.7}Al_{0.3}As$ QWs of widths $L = 100$ Å and $L = 500$ Å. Full curves correspond to the total magneto-absorption spectra.

essentially given by the valence cyclotron energy $\hbar\omega_v$. It is worthwhile to note that each nth Landau level contribution to the magneto-absorption spectra in figure 2 shows two features which may be related to structures [2] corresponding to on-centre and on-edge donors in the density of impurity states.

Also, for $B = 5$ T, and $L = 100$ Å, one clearly sees that the contribution for the total magneto-absorption due to transitions involving higher values of the Landau indices n decreases with increasing n. In the case of $L = 500$ Å the $n = 2$ contribution to the absorption spectra is barely seen. In fact, for higher applied magnetic fields this behaviour is even more pronounced: the calculated magneto-absorption for some other values of applied magnetic fields are shown in figure 3, where one clearly sees that transitions involving higher values of the valence Landau number n are smeared out as the field increases and the QW width increases, and this would *not* be observed in an actual experiment.

The dependence on the QW width of the peak position in the magneto-optical absorption spectra, associated with transitions involving the $n = 0$ valence Landau magnetic level, is displayed in figure 4(a) for applied magnetic fields of 0.1 T, 10 T, and 20 T, while the magnetic field dependence of the peak positions associated with the first few valence Landau levels is exhibited in figure 4(b) for QW widths of 100 Å and 500 Å. Notice that the peak positions corresponding to different Landau levels are essentially the same for small QW widths, as quantum confinement due to the barrier potential is more relevant than the effect of the applied magnetic field.

One should stress that the results presented in this work are somewhat qualitative, in the sense that the actual donor-related magneto-optical absorption spectra should be calculated taking into account a realistic valence-band structure [14]. Also, as the valence electron makes a transition to the shallow donor state it leaves a hole behind it, and in fact one has a physical system of an exciton which becomes bound to the shallow donor, and such excitonic effects are not included in the present approach.

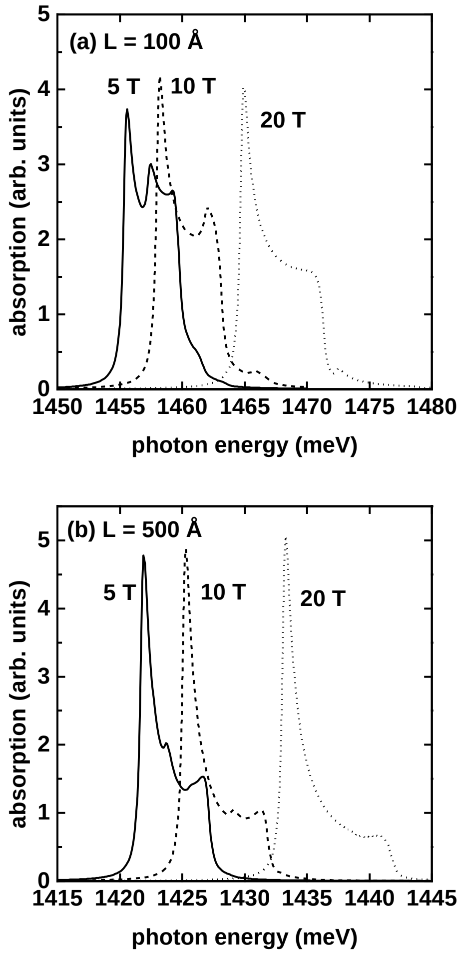

Figure 3. Magneto-optical absorption spectra associated with transitions from valence Landau magnetic levels to 1s-like donor states for various magnetic fields, and for (a) $L = 100$ Å and (b) $L = 500$ Å GaAs–$Ga_{0.7}Al_{0.3}As$ QWs.

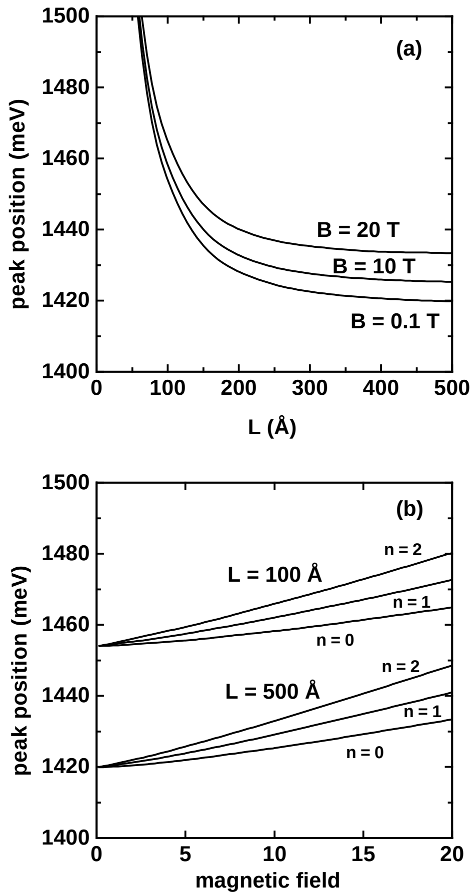

Figure 4. Peak positions of the magneto-absorption spectra for GaAs–$Ga_{0.7}Al_{0.3}As$ QWs, and associated with: (a) transitions from the $n = 0$ valence Landau level to 1s-like donor states as functions of the well width for different values of the applied magnetic field; (b) transitions from the $n = 0$, 1, and 2 valence Landau levels to 1s-like donor states as functions of the applied magnetic field, and for $L = 100$ Å and 500 Å QWs.

4. Conclusions

In conclusion, we have calculated the donor-related magneto-optical absorption spectra corresponding to transitions involving different valence Landau magnetic levels and donor states, and we have studied in detail the dependence of the magneto-absorption features for a range of QW widths, and applied magnetic fields. To our knowledge, there are no experimental measurements of impurity-related magneto-absorption in QWs to compare with our theoretical results. We believe, however, that the present study should stimulate experimental work in the area, and be of help in the quantitative understanding of forthcoming experiments.

Acknowledgments

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References

[1] Bastard G 1981 *Phys. Rev.* B **24** 4714
[2] Oliveira L E and Pérez-Alvarez R 1989 *Phys. Rev.* B **40** 10 460
Oliveira L E and López-Gondar J 1990 *Phys. Rev.* B **41** 3719
Oliveira L E and Mahan G D 1993 *Phys. Rev.* B **47** 2406
[3] Miller R C, Gossard A C, Tsang W T and Munteanu O 1982 *Phys. Rev.* B **25** 3871
[4] Shanabrook B V and Comas J 1984 *Surf. Sci.* **142** 504
Shanabrook B V, Comas J, Perry T A and Merlin R 1984 *Phys. Rev.* B **29** 7096
[5] Helm M, Peeters F M, DeRosa F, Colas E, Harbison J P and Florez L T 1991 *Phys. Rev.* B **43** 13 983
[6] Duffield T, Bhat R, Koza M, DeRosa F, Rush K M, and Allen S J Jr 1987 *Phys. Rev. Lett.* **59** 2693
Duffield T, Bhat R, Koza M, Hwang D M, DeRosa F, Grabbe P and Allen S J Jr 1988 *Solid State Commun.* **65** 1483
[7] Brozak G, de Andrade e Silva E A, Sham L J, DeRosa F, Miceli P, Schwarz S A, Harbison J P, Florez L T and Allen S J Jr 1990 *Phys. Rev. Lett.* **64** 471
[8] Belle G, Maan J C and Weimann G 1986 *Solid State Commun.* **56** 65
Belle G, Maan J C and Weimann G 1986 *Surf. Sci.* **170** 611
[9] de Dios-Leyva M and Galindo V 1993 *Phys. Rev.* B **48** 4516
[10] Brozak G, McCombe B D and Larsen D M 1989 *Phys. Rev.* B **40** 1265
[11] Skromme B J, Bhat R, Koza M A, Schwarz S A, Ravi T S and Hwang D M 1990 *Phys. Rev. Lett.* **65** 2050
[12] Strzalkowski I, Joshi S and Crowell C R 1976 *Appl. Phys. Lett.* **28** 350
[13] Wang W, Mendez E E and Stern F 1984 *Appl. Phys. Lett.* **45** 639
[14] Masselink W T, Chang Y-C and Morkoç H 1983 *Phys. Rev.* B **28** 7373
[15] White A M, Dean P J, Taylor L L, Clarke R C, Ashen D J and Mullin J P 1972 *J. Phys. C: Solid State Phys.* **5** 1727
[16] Latgé A, Porras-Montenegro N, de Dios-Leyva M and Oliveira L E 1996 *Phys. Rev.* B **53** 10 160
Barbosa L H M, Latgé A, de Dios-Leyva M and Oliveira L E 1996 *Solid State Commun.* **98** 215
Ribeiro F J, Latgé A and Oliveira L E 1996 *J. Appl. Phys.* **80** 2536
[17] Greene R L and Bajaj K K 1983 *Solid State Commun.* **45** 825
Greene R L and Bajaj K K 1985 *Phys. Rev.* B **31** 913
Greene R L and Bajaj K K 1986 *Phys. Rev.* B **34** 951
Greene R L and Bajaj K K 1988 *Phys. Rev.* B **37** 4604
Chaudhuri S and Bajaj K K 1984 *Solid State Commun.* **52** 967
Chaudhuri S and Bajaj K K 1984 *Phys. Rev.* B **29** 1803
[18] Shi J M, Peeters F M and Devreese J T 1994 *Phys. Rev.* B **50** 15 182
[19] Pérez-Alvarez R and Pajón-Suarez P 1988 *Phys. Status Solidi* b **147** 547
[20] Yoo B and McCombe B D 1991 *Phys. Rev.* B **44** 13 152