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Direct and indirect exciton mixing in a slightly asymmetric double quantum well

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Abstract. We studied, theoretically, the optical absorption spectra for a slightly asymmetric double quantum well (DQW), in the presence of electric and magnetic fields. Recent experimental results for a 10.18/3.82/9.61 nm GaAs/$Al_{0.33}Ga_{0.67}As$ DQW show clearly the different behaviours of the luminescence peaks for the indirect exciton IX and left direct exciton DX as functions of the external electric field. We show that the presence of a peak near the DX peak attributed to an impurity-bound left DX in the experimental results could be a consequence of non-trivial mixing between excitonic states.

1. Introduction

Theoretical study of excitons in double quantum wells began with the work of Kamizato and Matsuura [1]. They studied the excitonic levels and binding energies of symmetric wells as functions of the well and barrier widths. Dignam and Sipe [2] improved the calculation for the behaviour of the excitonic levels for wide barriers, incorporating the Coulomb interaction between excitonic states. Their work included both symmetric and asymmetric GaAs/$Al_{0.33}Ga_{0.67}As$ wells (see also reference [3]). For similar studies for other materials see reference [4] and reference [5], and for reviews of this subject see reference [6] and reference [7]. For a recent theoretical discussion see reference [8] and references therein, and for a recent experimental discussion see reference [9].

In this work, we have studied the excitonic energy levels in an asymmetric vertical double quantum well as functions of the magnetic and electric field strengths. Within the effective-mass approach we expanded the excitonic wave function in an orthogonal basis formed by products of electron and hole wave functions along the crystal growth direction $\vec{z}$, and one-particle solutions of the magnetic Hamiltonian in the x–y plane. The Coulomb potential between electrons and holes produces off-diagonal terms, thus mixing our basis states. We obtained the energy spectra and wave functions by diagonalizing the excitonic Hamiltonian in a truncated basis. We applied our method to study the excitonic states in a GaAs/$Al_{0.33}Ga_{0.67}As$ DQW, for the specific case of a DQW composed of a left well of 10.18 nm, a barrier of 3.82 nm, and a right well of 9.61 nm. The effects of external electric and magnetic fields on the luminescence (PL) intensity for this heterostructure have recently been studied experimentally by Krivolapchuk *et al* [10, 11].

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2. Formalism

The effective-mass Hamiltonian for excitons in a double quantum well in the diagonal approximation [6] and in the presence of a magnetic field pointing in the z-direction can be written as

$$H = H_0(z_e) + H_0(z_h) + H_{mag}(r) + V_{coul}(r, |z_e - z_h|) \tag{1}$$

where $H_0(z_e)$ is the one-dimensional Hamiltonian for electrons:

$$H_0(z_e) = p_{ze}^2/2m_{ze} + V_e(z_e) \tag{2}$$

and $H_0(z_h)$ is the one-dimensional Hamiltonian for holes:

$$H_0(z_h) = p_{zh}^2/2m_{zh} + V_h(z_h) \tag{3}$$

and where $V_e(z_e)$ ($V_h(z_h)$) is the potential that defines the double quantum well for electrons (holes) in the five regions of z. We included the electric field in $V_e(z_e)$ and $V_h(z_h)$ by a shift in the potential in steps similar to that in figure 1. $H_{mag}(r)$ is the magnetic Hamiltonian in the symmetric gauge, which depends on the relative coordinates of electrons and holes in the x–y plane:

$$H_{mag} = \frac{(\vec{p} - q\vec{A})^2}{2\mu} + \frac{qB}{m_{h,x-y}} l_z \tag{4}$$

where $\vec{p}$, μ, and $m_{h,x-y}$ are the momentum operator, reduced mass, and hole mass respectively, defined on the x–y plane, q is the electron charge $-|e|$, and B is the magnetic field.

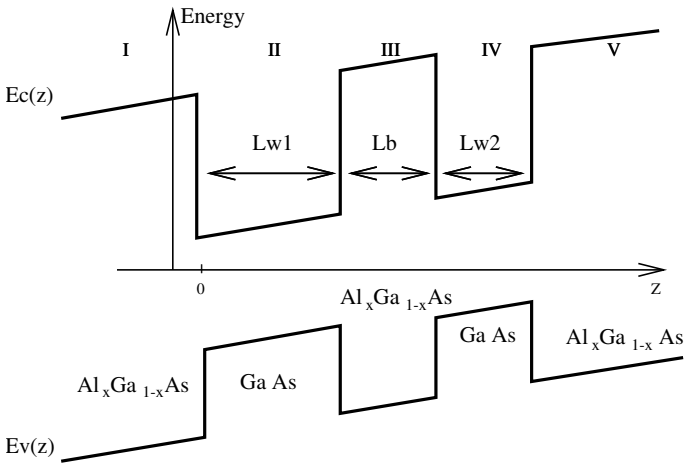

Figure 1. Potential profiles along the z-direction for electrons and holes.

$V_{coul}(r, |z_e - z_h|)$ is the Coulomb potential between electrons and holes, including an effective dielectric constant for the system.

We expanded the solutions of the Hamiltonian (1), as a linear combination of products of eigenfunctions of the magnetic Hamiltonian in the x–y plane (4), and eigenfunctions of the electron and hole Hamiltonians in the z-direction ((2) and (3)):

$$\Psi_n^{exc} = \sum_{\nu_r, \nu_e, \nu_h} C^n_{\nu_r, \nu_e, \nu_h} \psi_{\nu_r}(r, \phi) \psi_{\nu_e}(z_e) \psi_{\nu_h}(z_h) \tag{5}$$

in which, in the symmetric gauge,

$$\psi_{\nu_r,l} = \frac{1}{2\pi}\left(\frac{2(\nu_r - l/2 - |l|/2)g_B^{|l|+1}}{(|l|/2+\nu_r - l/2)!}\right)^{1/2} \mathrm{e}^{\mathrm{i}l\phi}\left(\frac{r}{\mathrm{i}}\right)^{|l|} \mathrm{e}^{-g_B r^2/2} L^{|l|}_{\nu_r - l/2 - |l|/2}(g_B r^2) \tag{6}$$

where $g_B = qB/(2\hbar)$, and only $l = 0$ functions are considered. The electron wave functions defined in the five regions of z, shown in figure 1, are given in terms of $\sin(z_e)$, $\cos(z_e)$, and $\pm\exp(z_e)$. The hole wave functions are given by similar expressions.

The Coulomb interaction produces off-diagonal terms by mixing our basis states. In order to obtain the system of equations for the coefficients in expansion (5), we need to evaluate the Coulomb integrals

$$\int \mathrm{d}\phi\ \mathrm{d}r\ \mathrm{d}z_e\ \mathrm{d}z_h\ \psi^*_{\nu_r'}\psi_{\nu_e'}\psi_{\nu_h'}V_{coul}(r, |z_e - z_h|)\psi_{\nu_r}\psi_{\nu_e}\psi_{\nu_h}. \tag{7}$$

The ϕ-integral is trivial, because of l_z-conservation. Using the explicit expansion of the Laguerre polynomials (L_n) of $\psi_{\nu_r'}$ and ψ_{ν_r} (6), and after solving the r-integral, equation (7) can be written as a sum of terms of the form

$$\int_0^\infty \mathrm{d}\alpha \left(\frac{\alpha^2}{4g_B}\right)^m \mathrm{e}^{-\alpha^2/(4g_B)} \int_{-\infty}^{\infty} \mathrm{d}z_e\ \mathrm{d}z_h\ \psi_{\nu_e'}\psi_{\nu_h'}\mathrm{e}^{-|z_e - z_h|\alpha}\psi_{\nu_e}\psi_{\nu_h}. \tag{8}$$

The z_e- and z_h-integrals can be solved analytically. The evaluation of these integrals is complicated due to the large number of terms, resulting from the five different regions of the potential. The z_e- and z_h-integrals contain both decoupled terms in which the z_e- and z_h-integrals are independent of each other and coupled terms where the integration limits of the z_h-integral contain z_e. The remaining α-integral must be calculated numerically.

By diagonalizing the system of equations resulting for the coefficients in expansion (5), in a truncated basis, we obtained the energies and wave functions for the first excitonic levels. Evaluating the oscillator strength we obtained the optical absorption spectra.

We have previously used this method of calculation [12] for zero electric field, to study the excitonic binding energy and optical absorption for type I symmetric and asymmetric double quantum wells, as functions of magnetic field, and of barrier and well widths. In that work our method was tested and compared to other work; excellent agreement with previously known results was obtained.

3. Results

We calculated the excitonic energy levels for a slightly asymmetric 10.18/3.82/9.61 nm GaAs/$Al_{0.33}Ga_{0.67}$As double quantum well, in the presence of electric and magnetic fields. The band gap used in our calculations is given by $E_g(x) = 1.52 + 1.36x + 0.22x^2$ ($x = 0.33$). The band-gap offset considered was 60% for the conduction band and 40% for the valence band. For all five regions in the double quantum well, we used the same electronic mass $m_e = 0.067m_0$, the x–y plane heavy-hole mass $m_{hh,x-y} = 0.1m_0$, the z-axis heavy-hole mass $m_{hh,z} = 0.45m_0$, the light-hole masses $m_{lh,x-y} = 0.2m_0$ and $m_{lh,z} = 0.08m_0$, and a dielectric constant $\epsilon = 12.5\epsilon_0$. In our calculations we used a truncated basis set composed of 12 Landau wave functions, four electronic wave functions, and five heavy-hole wave functions, for which most of our results converged to less than a tenth of a meV. For magnetic fields below 5 T, we would need to increase the number of Landau levels considered. We included a fictitious width of 1.5 meV for each optical absorption peak.

3.1. Energies and wave functions for electrons and holes

In this section we present our results for the energies and wave functions of electron and holes in a one-dimensional DQW, as a function of the external electric field. We are interested in regions of electric field where two different electron (or hole) energy levels cross each other leaving a gap of a few meV between them. When the wave functions involved in this kind of anticrossing are important for the optical absorption, we expect to find interesting behaviours of the peaks of the excitonic optical absorption.

Figure 2 shows the electron (upper plot) and hole (lower plot) energy levels for this DQW as functions of the external electric field. In the range from 0 to 60 kV cm^{-1} (not shown in the plot), there are crossings in the hole energy levels near 5, 15, 25, and 40 kV cm^{-1}. These crossings do not meet the two conditions explained before, and will not produce a noticeable behaviour of the excitonic optical absorption. In the range from 60 to 85 kV cm^{-1} there is a region of electric fields near 67 kV cm^{-1}, indicated with an arrow, where the second and the third electronic energy levels anticross. To understand the excitonic optical absorption it is necessary to know the behaviour of the electron and hole DQW wave functions for electric field below, inside, and above the anticrossing region.

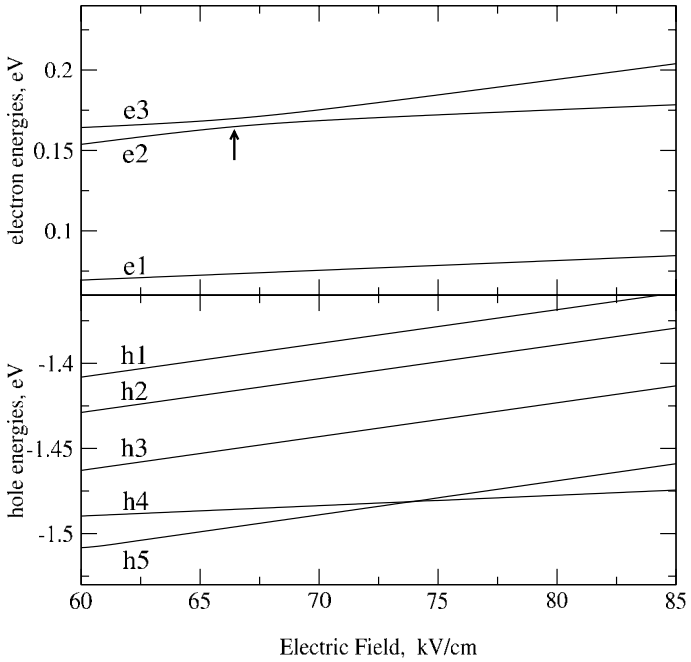

Figure 2. One-dimensional electron (top) and hole (bottom) energy levels in a 10.18/3.82/9.61 nm $GaAs/Al_{0.33}Ga_{0.67}As/GaAs$ DQW as a function of the electric field strength.

Figure 3 shows the first four electron (upper plot) and hole (lower plot) wave functions for zero external electric field. Numbers indicate the orders of the energy levels, and the most important states for the excitonic optical absorption are represented by solid lines. The first state mostly localized in the left (wider) well is called **L1** and the first state mostly localized in the right well is called **R1**. It is clear from this figure that holes are almost completely localized in the left or right wells, and that electrons have strong components over both wells. This difference in behaviour for electrons and holes is a consequence of the effective-mass

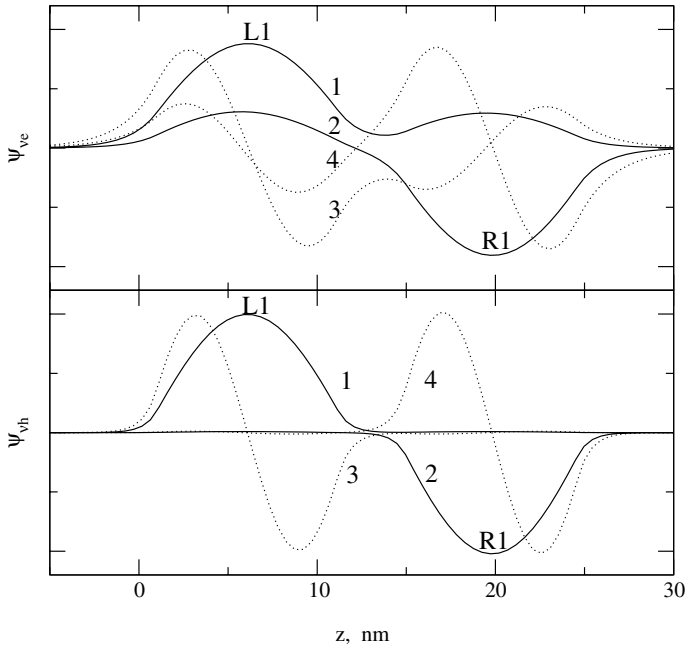

Figure 3. One-dimensional electron and hole wave functions in the DQW for zero electric field. The upper plot corresponds to electrons and the lower plot to holes; numbers represent the orders of the energy levels, and the letter L (R) indicates that the state is mostly localized in the left (right) quantum well. $z = 1$ corresponds to the beginning of the first QW.

differences for electron and holes and the size of the wells and barrier in this sample.

Figure 4 shows the electron (upper plot) and hole (lower plot) wave functions for an external electric field of 71 kV cm^{-1}, where the most important states for the excitonic optical absorption are represented by solid lines. Comparing with the previous case of electrons in zero electric field, we note that: the first level **L1** gets much more localized in the left well, the second level **R1** changes dramatically into **L2**, and the third level behaves as **R1**. For holes we can see that the electric field forces the wave functions to be localized in the right well, and the fourth level is localized in the left well (corresponding to **L1**).

Figure 5 shows the electron (upper plot) and hole (lower plot) wave functions for an external electric field of 85 kV cm^{-1}. Again the most important states for the excitonic optical absorption are represented by solid lines. Comparing with the previous case of a 71 kV cm^{-1} electric field, we note that electron wave functions remain almost unchanged, and that the fifth hole wave function behaves as **L1**.

In order to understand better the excitonic behaviour and the optical absorption spectra, it is also possible to calculate the expectation values $\langle z_e \rangle_n$, $\langle z_h \rangle_n$, and $\langle \rho_e \rangle_n$ as functions of the electric and magnetic fields using the excitonic wave function (5), but at present we have not incorporated these calculations in our numerical routines.

3.2. Optical absorption as a function of the electric field

Increasing the electric field in a double quantum well produces a shift in the electron and hole energy levels and a change in the localization of the respective wave functions. The combination of the two effects changes the behaviour of the excitonic states and affects, in a

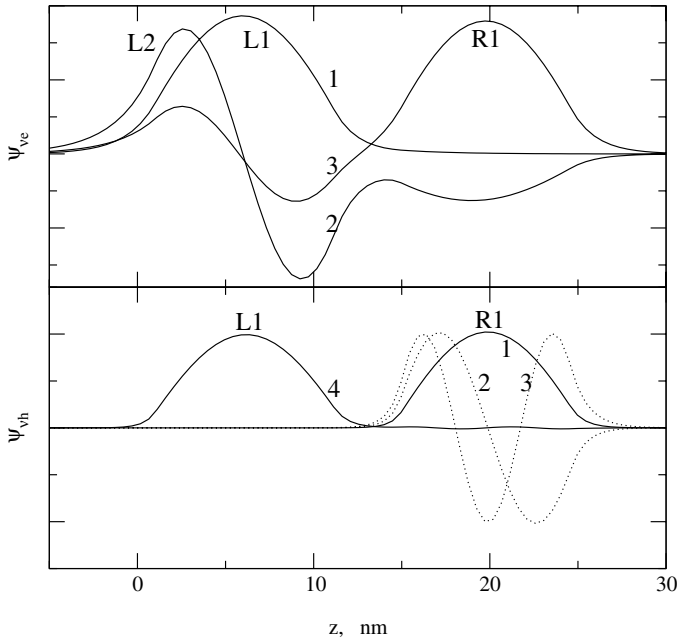

Figure 4. One-dimensional electron and hole wave functions in the DQW for an electric field of 71 kV cm^{-1}. The upper plot corresponds to electrons and the lower plot to holes; numbers represent the orders of the energy levels, and the letter L (R) indicates that the state is mostly localized in the left (right) quantum well. $z = 1$ corresponds to the beginning of the first QW.

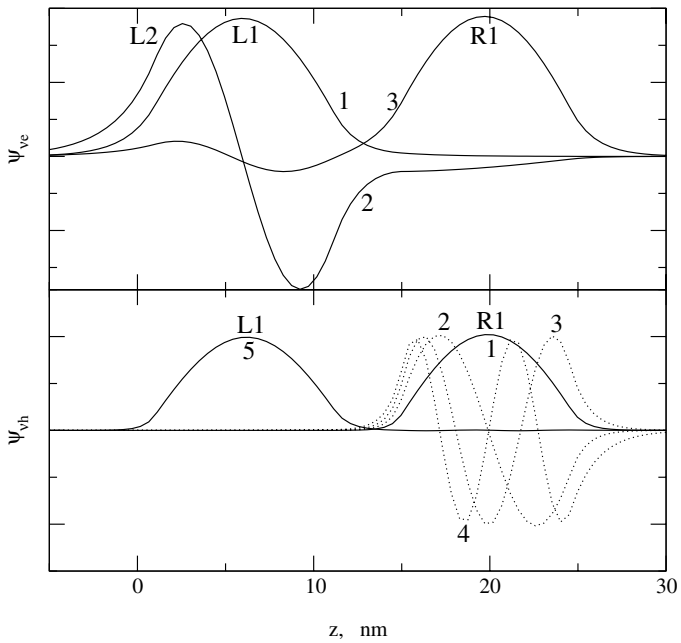

Figure 5. One-dimensional electron and hole wave functions in the DQW for an electric field of 85 kV cm^{-1}. The upper plot corresponds to electrons and the lower plot to holes; numbers represent the orders of the energy levels, and the letter L (R) indicates that the state is mostly localized in the left (right) quantum well. $z = 1$ corresponds to the beginning of the first QW.

non-trivial way, the optical absorption spectrum of these systems.

Figure 6 shows the electric field effects on the optical absorption spectra for an external magnetic field of 10 T. Each curve, corresponding to a different value of the electric field, has been displaced for clarity. For an electric field of 60 kV cm^{-1} (upper curve) there are two peaks in the excitonic optical absorption. The first peak corresponds to a direct exciton **L1L1**, where the constituent electron and hole are localized in the left (wider) well. The second peak corresponds to a direct exciton **R1R1**, where the electron and hole are localized in the right well. For an electric field of 85 kV cm^{-1} (lower curve) the same two peaks occur, corresponding again to the left direct exciton **L1L1** and the right direct exciton **R1R1**. The main difference between the 60 kV cm^{-1} and the 85 kV cm^{-1} case is in the exciton composition in terms of the basis states. This difference in composition of basis states cannot be observed experimentally in the previous limiting cases, but has a strong influence on the optical absorption behaviour for electric fields between 60 kV cm^{-1} and 85 kV cm^{-1}. The complex structure in the optical absorption spectra in this range of electric fields can be explained by the formation of excitonic states, which have a strong component of indirect exciton states. In this case the indirect exciton state corresponds to **L2R1**, which is formed by an electron in the second left state and a hole in first right state. The composition in terms of our basis states can be obtained from figures 3, 4, and 5. When comparing figure 6 with figure 2 of [10], we see similar behaviours of the PL peaks. This suggests that the peak attributed to an impurity-bound direct exciton in the experimental results could be interpreted as a mixed state with direct and indirect exciton components. Quantitative agreement between our results and those from the experimental work is not possible because we included a strong magnetic field. Peaks originating from light-hole states appear on the right of this figure (not shown).

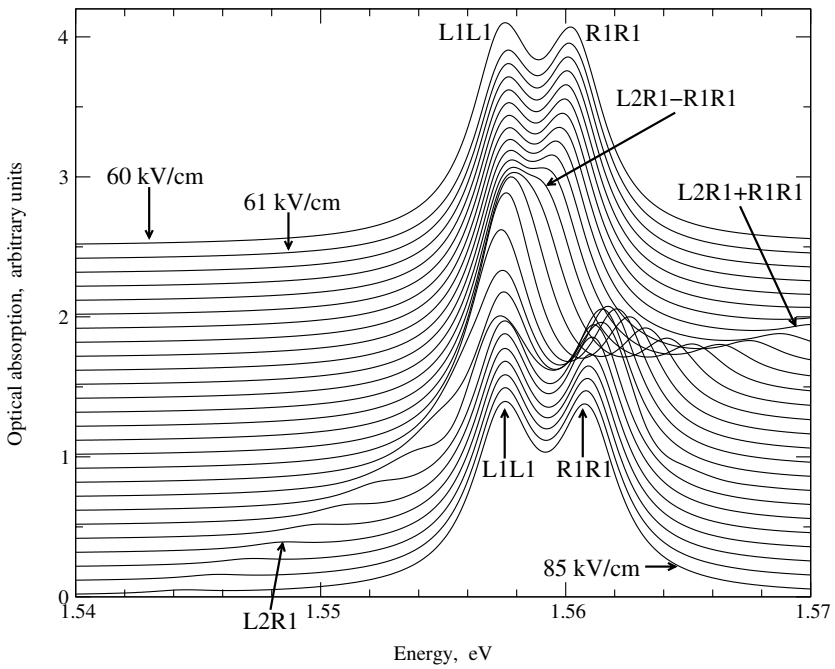

Figure 6. Optical absorption spectra for this DQW for a 10 T magnetic field and electric fields ranging from 60 kV cm^{-1} (upper curve) to 85 kV cm^{-1} (lower curve). Labels indicate the main composition for each electron–hole excitonic pair; the letter L (R) indicates that the electron or hole state is mostly localized in the left (right) quantum well.

3.3. Optical absorption as a function of magnetic field

Increasing the magnetic field in a double quantum well produces a shift in the excitonic energy levels towards higher energies and an increase in the interaction energy. The increase in the energy of interaction between electrons and holes is a consequence of two effects. First, the wave-function confinement in the x–y plane produces a stronger interaction along the z-direction, as the wave functions penetrate more into the barrier. Second, the interaction between electrons and holes in the same plane increases, because their wave functions are confined to a smaller region.

Figure 7 shows the magnetic field effects on the optical absorption spectra for an external electric field of 71 kV cm^{-1}. The differences in the interaction energies in the layer plane and along the z-axis when the magnetic field is varied produce different behaviours of the optical absorption peaks with direct and indirect exciton components. This difference produces the splitting of the first peak for a magnetic field of 5 T into two peaks for stronger magnetic fields.

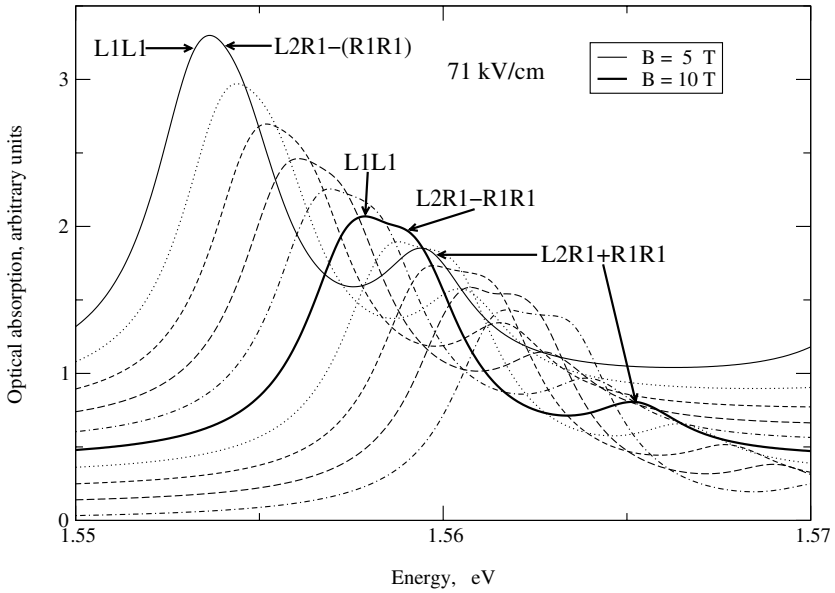

Figure 7. Optical absorption spectra for this DQW for a 71 kV cm^{-1} electric field and the magnetic field ranging from 5 T (upper curve) to 14 T (lower curve). Labels inside parentheses indicate the small contributions from these states to the total excitonic wave function.

Figure 8 shows the magnetic field effects on the optical absorption spectra for an external electric field of 78 kV cm^{-1}. In this case the magnetic field produces no mixing between excitonic states, and produces different shifts in energies for direct excitons (**L1L1** and **R1R1**) and the indirect exciton (**L2R1**). This effect is clearly observed as a function of magnetic field.

4. Conclusions

In this work we studied the energies and wave functions of excitonic states in a 10.18/3.82/9.61 nm GaAs/$Al_{0.33}Ga_{0.67}As$ double quantum well, in a magnetic field pointing along the growth direction $\vec{z}$. We calculated the optical absorption spectra as functions of the external electric and magnetic fields and studied the behaviour of the PL peaks for the indirect exciton IX and direct exciton DX. We compared our results and those in the experimental work

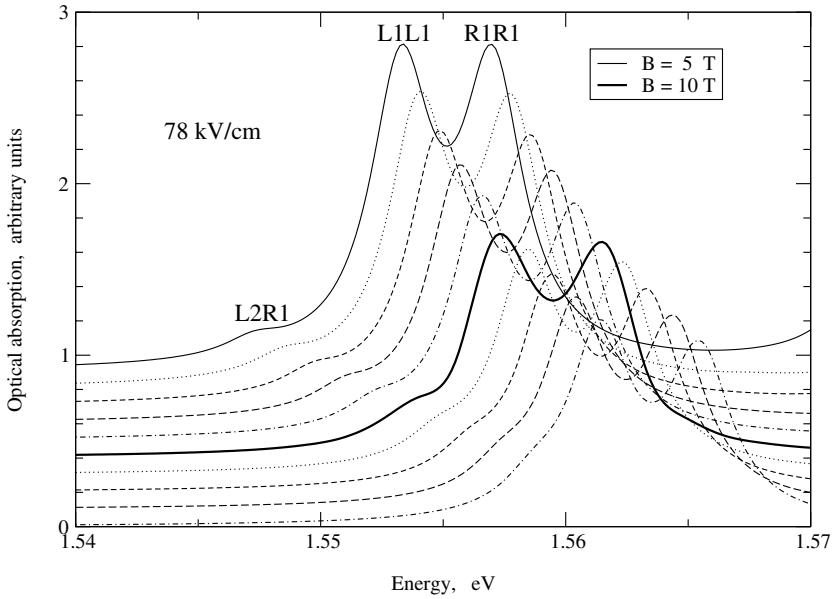

Figure 8. Optical absorption spectra for this DQW for a 78 kV cm^{-1} electric field and the magnetic field ranging from 5 T (upper curve) to 14 T (lower curve).

of [10] and found similar behaviours of the PL peaks. This suggests that the peak attributed to an impurity-bound direct exciton in the experimental results could be interpreted as a mixed state with direct and indirect exciton components. The indirect exciton peak component behaves differently to those for a direct exciton and an impurity-bound direct exciton when the magnetic field is varied. This difference in behaviour could be detected experimentally, and would permit clear identification of the compositions of these mixed excitonic states.

In our method of calculation we used an orthogonal basis that involves functions of single-particle solutions of the double quantum well in the z-direction, which makes our method appropriate for small and medium barrier widths. The study of these systems for magnetic fields below 5 T within this method requires increase of the number of Landau levels in our basis states, making the numerical computation excessively time consuming.

Acknowledgments

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