Direct and indirect excitons in asymmetric double quantum wells

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We studied, theoretically, the optical absorption spectra for asymmetric double quantum wells, in the presence of electric and magnetic fields. Recent experimental results show clearly the different behavior in the luminescence peaks for the indirect exciton IX and left direct exciton DX as a function 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 the non-trivial mixing between excitonic states.

Keywords: Quantum wells, excitons, low dimensional systems.

En este trabajo estudiamos teóricamente el espectro de absorción óptica de pozos cuánticos dobles asimétricos en presencia de campos eléctricos y magnéticos. Los resultados experimentales recientes muestran claramente la conducta diferente de los peaks de luminescencia para el excitón indirecto IX y para el excitón izquierdo directo DX, en función del campo eléctrico externo. Aquí mostramos que la presencia de un peak cercano al peak del DX, el cual fue atribuido a un estado de impureza ligado al DX izquierdo en los resultados experimentales, puede ser una consecuencia de la mezcla no trivial entre estados excitónicos.

Descriptores: Pozos cuánticos, excitones, sistemas de baja dimensión.

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Introduction

In this work we studied the excitonic energy levels in an asymmetric vertical double quantum well (DQW) as a function 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 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 energy levels. Evaluating the oscillator strength we obtained the optical absorption spectra.

Model

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

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

where \( H_0(z_e) \) is the one-dimensional Hamiltonian for electrons, \( H_0(z_h) \) is the one-dimensional Hamiltonian for holes, and \( V_c(z_e) \) is the potential that defines the double quantum well for electrons (holes) in the five regions of z. We included the electric field in \( V_c(z_e) \) and \( V_h(z_h) \) by a shift in the potential in stair steps. \( H_{mag}(r) \) is the magnetic Hamiltonian in the symmetric gauge, which depends on the relative coordinates of electrons and holes in the x - y plane, \( V_{coul}(r, |z_e - z_h|) \) 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, and eigenfunctions of the electron and hole Hamiltonians in the z direction,

\[ \psi_{n}^{exc} = \sum_{\nu_e, \nu_h, \nu_z} C_{\nu_e, \nu_h, \nu_z}^{n} \psi_{\nu_e}(r, \phi)\psi_{\nu_h}(z_e)\psi_{\nu_z}(z_h), \] (2)

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 (2), we need to evaluate the Coulomb integrals

\[ \int d\phi dr dz_e dz_h \psi_{\nu_e}^{*} \psi_{\nu_h}^{*} \psi_{\nu_e} \psi_{\nu_h} \times V_{coul}(r, |z_e - z_h|) \psi_{\nu_e} \psi_{\nu_h}. \] (3)

By diagonalizing the system of equations resulting for the coefficients in expansion (2), 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.
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

\[ E_g(x) = 1.52 + 1.36x + 0.22x^2 \quad (x = 0.33). \]

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 magnetic field of 10 T, a truncated basis set composed of 12 Landau wave functions, four electronic wave functions, five heavy-hole wave functions, for which most of our results converged to less than a tenth of meV. The method becomes unsuitable for low magnetic fields, since then we would need to use a prohibitively large number of Landau levels. We included a fictitious width of 1.5 meV for each optical absorption peak.

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 both effects changes the behavior of the excitonic states and affects, in a non trivial way, the optical absorption spectra in this range of electric fields.

Figure 1 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 (upper curve) there are two peaks in the excitonic optical absorption. The first peak corresponds to a direct exciton \(L_1L_1\), where the constituent electron and hole are localized in the left (wider) well. The second peak corresponds to a direct exciton \(R_1R_1\), where the electron and hole are localized in the right well. For an electric field of 85 kV/cm (lower curve) the same two peaks occur, corresponding again to the left direct exciton \(L_1L_1\) and the right direct exciton \(R_1R_1\). The main difference between the 60 kV/cm and the 85 kV/cm case is the exciton composition in terms of the base states. This different composition of base states can not be

![Figure 1. Optical absorption spectra for this DQW for a 10 Tesla magnetic field and electric fields ranging from 60 kV/cm (upper curve) to 85 kV/cm (lower curve). Labels indicate the main composition of the electron-hole excitonic pair, letter L (R) indicates that the electron or hole state is mostly localized in the left (right) quantum well.](image)

observed experimentally in the previous limiting cases, but has a strong influence in the optical absorption behavior for electric fields between 60 kV/cm and 85 kV/cm. 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 excitons. In this case the indirect exciton state corresponds to \(L_2R_1\), which is formed by an electron in the second left state and a hole in first right state. When comparing this figure with Fig. 2 of Ref. [1], we see a similar behavior in 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 in the experimental work is not possible because we included a strong magnetic field. Peaks originating from light holes states appear at the right end of this figure (not shown).

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