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**FINE STRUCTURE OF EXCITONS IN QUANTUM WELLS**

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Nous présentons une analyse théorique de la structure fine des excitons dans les puits quantiques qui prend conjointement en compte, le Rydberg effectif, l'échange électron-trou et la multiplicité de spin. Ce modèle nous permet d'analyser quantitativement des résultats expérimentaux obtenus pour des structures GaAs-Ga<sub>0.5</sub>Al<sub>0.5</sub>As.

We present a theoretical investigation of the fine structure for quantized exciton including effective Rydberg, electron hole exchange interaction and spin multiplicity which enables to analyze experimental results earlier reported for GaAs-Ga<sub>0.5</sub>Al<sub>0.5</sub>As.

I - Introduction

Free excitons are excited electronic states of the crystal which have been observed for a long time in 3D compounds and more recently in 2D systems. In the case of type I quantum wells (QW) we will show that the spatial confinement of the electrons in the z direction simultaneously influences the effective Rydberg, as already established [1] but also leads to a drastic enhancement of the electron hole exchange interaction (EHEXI) which has never been theoretically considered hitherto.

II - Basic equations

We first express the wave function of the non degenerate confined exciton in the envelope function framework. Neglecting the spin multiplicity it writes :

$$\psi = 1/\sqrt{A} e^{iKR} \varphi^{2D}(\vec{r}_e - \vec{r}_h) \chi_e(z_e) \chi_h(z_h) U_{c,o}(r_e) U_{v,o}(r_h) \quad (1)$$

where A is the area, K and R the in plane wave vector and coordinate of the center of mass.  $\varphi^{2D}$  a quasi 2D envelope function,  $\chi_i$  and  $U_{i,o}$  the solution of the square well problem and Bloch function respectively. After some algebraic manipulations which have been detailed elsewhere [2], using the parameters characteristics of a 3D exciton with Bohr radius  $a_0^*$  one can express the short range part of EHEXI as follows for the ground state of the exciton :

$$\epsilon_{ex}^{2D} = (\pi a_0^{*3}) \epsilon_{ex}^{3D} \omega_{eh} |\varphi^{2D}(o)|^2 \quad (2)$$

Here  $\epsilon_{ex}^{2D}$  is EHEXI for the bulk. Most of the contribution to  $\epsilon_{ex}^{2D}$  arise when both electron and hole are located in a same cell ; this is accounted for by the joint probability :

$$\omega_{eh} = \int_{-\infty}^{+\infty} \chi_e^2(z) \chi_h^2(z) dz. \quad (3)$$

Similarly the longitudinal transverse splitting (long range part of EHEXI) is given by

$$E_{LT}^{2D} = (\pi a_0^{*3}) E_{LT}^{3D} \omega_{eh} |\varphi^{2D}(o)|^2. \quad (4)$$

III - THE GaAs-Ga<sub>0.5</sub>Al<sub>0.5</sub>As case

We first suppose for simplicity that, in the range of our numerical investigation, EHEXI has a small enough influence on the confinement of the exciton wave function, to keep valid the perturbation treatment. Next, to calculate the transition energies without EHEXI we make the approximation of decoupled heavy and light hole subbands. Taking into account of the influence of mass mismatch and the non parabolicity effect, the binding energies have been calculated for both heavy hole and light hole excitons as a function of the well width, using a variational approach similar to the one of Greene and Bajaj [1], but using a set of gaussians as trial function. Third we have to express the exchange interaction on the exciton basis  $|m_h, m_s\rangle$  where  $m_h$  and  $m_s$  are the z components of the hole  $J = 3/2$  and electron  $S = 1/2$  angular momentum. In 3D case, and in a spherical approximation, the exchange hamiltonian is written [3] :

$$H = \epsilon^{3D}_{ex}/6 (3-4 \vec{J} \cdot \vec{S}) \quad (5).$$

In the case of a QW we have to take into account of the difference between the envelope functions, joint probabilities for heavy hole excitons (HHE) and light hole excitons. So let  $\Delta_h = 4/3 \epsilon^{2D}_{ex}$  (HHE),  $\Delta_l = 4/3 \epsilon^{2D}_{ex}$  (LHE) and

$$\Delta_{hl} = \omega_{eh}^{hl} [\Delta_h \Delta_l / (\omega_{eh}^{hh} \omega_{eh}^{ll})]^{1/2}$$

$$(\omega_{eh}^{ij} \text{ is given by : } \int_{-\infty}^{+\infty} x^2 e(z) x^i_h(z) x^j_h(z) dz).$$

The longitudinal transverse splitting corresponds to a shift toward high energy of the longitudinal spin singlet Wannier exciton [4].

The total hamiltonian writes :

| $ \pm 3/2, \pm 1/2\rangle$ | $ \pm 3/2, \mp 1/2\rangle$          | $ \pm 1/2, \pm 1/2\rangle$          | $ +1/2, -1/2\rangle$                        | $ -1/2, +1/2\rangle$                        |
|----------------------------|-------------------------------------|-------------------------------------|---|---|
| $E_h$                      | 0                                   | 0                                   | 0   | 0   |
| 0                          | $E_h + \frac{3}{4}\Delta_h$         | $\mp \frac{\sqrt{3}}{4}\Delta_{hl}$ | 0   | 0   |
| 0                          | $\mp \frac{\sqrt{3}}{4}\Delta_{hl}$ | $E_l + \frac{3}{4}\Delta_l$         | 0   | 0   |
| 0                          | 0                                   | 0                                   | $E_l + \frac{1}{2}(\Delta_l + E_{LT}^{2D})$ | $-\frac{1}{2}(\Delta_l + E_{LT}^{2D})$      |
| 0                          | 0                                   | 0                                   | $-\frac{1}{2}(\Delta_l + E_{LT}^{2D})$      | $E_l + \frac{1}{2}(\Delta_l + E_{LT}^{2D})$ |

The low energy heavy hole exciton  $|\pm 3/2, \pm 1/2\rangle$  has a dipole forbidden symmetry. The left hand block diagonal matrix correspond to  $\sigma$ -allowed recombinations (E1 001) while the only dipole allowed state in the right hand matrix is the antisymmetric combination of  $|1/2, -1/2\rangle$  and  $|-1/2, 1/2\rangle$ , the polarization of the corresponding light is  $\pi$ .  $E_h$  and  $E_l$  represent the heavy hole and light hole exciton transition energies without EHEXI.

IV - NUMERICAL CALCULATION

A numerical calculation made for two series of the aluminium context  $x = 0.3$  and  $x = 0.5$  using a valence band off set of 33% of the gap mismatch give us the results gathered on figure 1 (the energy is expressed as a function of  $\epsilon^{3D}_{ex}$  and the 3D Bohr radius is used to measure the well width). It is worth noting that the behavior of EHEXI resembles the Rydberg ones but it is much more strongly enhanced. (Remember that a maximum value of four is found in the true 2D case [5]). Now we want to give an experimental support to this calculation ; this can be done using the photoluminescence results reported in the work of Bauer et al [6] which observed a doublet structure on the heavy hole exciton states in a series of high purity GaAs-Ga<sub>0.5</sub>Al<sub>0.5</sub>As QWs with different widths. This doublet structure concerns

dipole forbidden and dipole allowed heavy hole type excitons ; the dipole forbidden transition can be observed in luminescence because of thermalization. As it is displayed on figure 2, our calculation where no adjustable parameter has been included (we used the bulk GaAs values) fits the experimental data. For very narrow well width the decrease of the calculated splitting leads to a small discrepancy with respect to the experiments. The reasons for such disagreement is not clear. The influence of in-plane and in-axis masses is illustrated on figures 3 and 4. Figure 3 displays the change in  $|\varphi^{2D}(0)|^2$  for HHE and LHE in the case of aluminium contents  $x = 0.3$  and  $x = 0.5$ . Since the in plane mass is higher for LHE than for HHE, the exciton wave function is less delocalized in the latter case than in the former. Comparing both  $x = 0.3$  and  $x = 0.5$ , one evidences the influence of the well depth on the confinement. Finally one expected larger values for  $\omega_{eh}$  when considering HHE instead of LHE because of the relative magnitude of in axis masses ; this has been found as shown in figure 4. In the case of type II quantum wells both  $\Delta_h$  and  $\Delta_l$  are expected to be very small.

FIGURE 1 : Well width dependence of the exchange energy for GaAs-Ga<sub>1-x</sub>Al<sub>x</sub>As quantum wells with aluminium contents  $x = 0.3$  and  $x = 0.5$ . The solid lines corresponds to the heavy hole excitons, the dashed line correspond to light hole excitons.

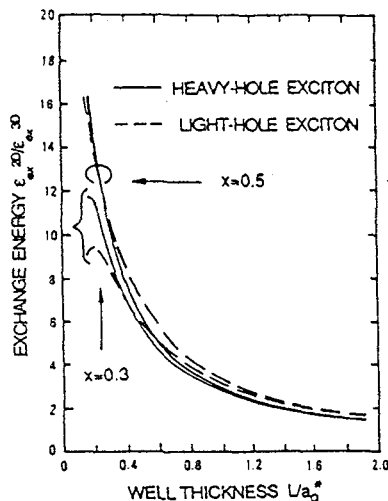


FIGURE 2 : Well width dependence of the exchange splitting of the heavy hole exciton for GaAs-Ga<sub>0.5</sub>Al<sub>0.5</sub>As QWs. The solid line is the calculation. The experimental points are taken from Ref. 6.

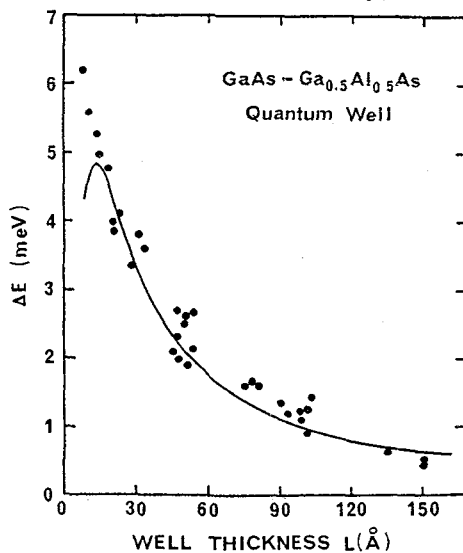


FIGURE 3 : Change in  $|\psi^{2D}(0)|^2$  with the aluminium content and well width. The dashed line corresponds to light hole excitons, the full line to heavy hole excitons. The influence of mass mismatches between the confining layer and the barrier have been taken into account.

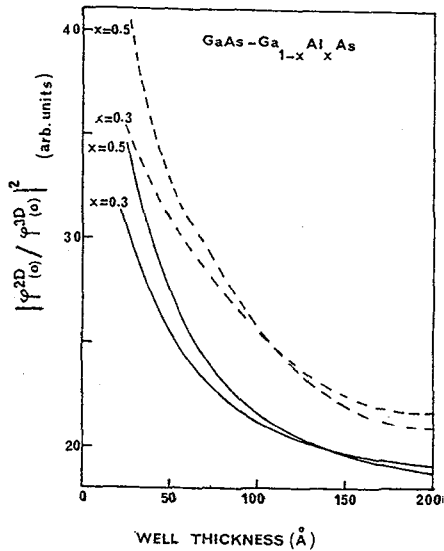
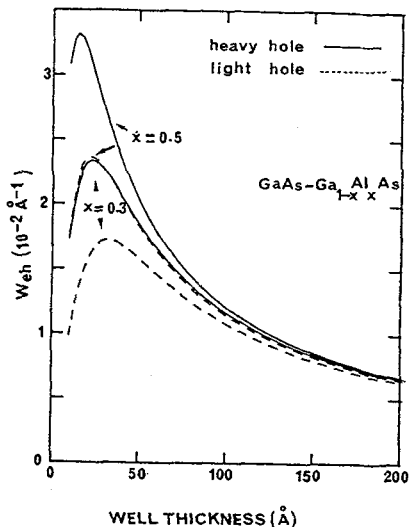


FIGURE 4 : The variation of the joint probability as a function of the barrier heights and well-width. The calculation has been made with a valence band offset of 33 percents of the gap mismatch, according with ref [7]

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