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Abstract : We present the results of a variational calculation of the ground state energy of a (D^+, X) complex in a quantum well with finite potential barriers as a function of the depth and the width of the well as well as the ratio σ of the electron and hole effective masses. We use the envelope function approximation. We apply our results to the system $GaAs/Ga_{1-x}Al_xAs$ with x = 0.15 and x = 0.30. It appears that the coulombic correlation energy goes through a minimum for a well thickness in the order of 50 Angströms. This minimum is comprized between the values obtained in the 2D and 3D limit cases. Furthermore, it appears that only the heavy hole states give rise to a stable binding energy for all values of the well thickness. The light hole states give rise to stable binding only in the case of large thicknesses.

1. INTRODUCTION

The properties of excitons bound to neutral or ionized impurities have been extensively studied[1,2] during the last years. They have been observed in many semiconductors since the early 1960s. The bound exciton states are very common because most practical semiconductors contain in significant quantity impurities or defects which can produce this binding. The binding energy of the exciton to the impurity or defect is generally weak compared to the free-exciton binding energy. Moreover, it is now well known that if neutral centres should always exhibit a finite binding energy,[3] the ionized donors or acceptors should only bind excitons under special circumstances.[4,16] The recent advances in the crystal growth technique of molecular epitaxy allow the engineering of semiconductors on an atomic scale such as superlattices or quantum wells (QW's).[5] In these heterostructures the quantum confinement effects may become important. In particular the coulombic interaction between electrons and holes is increased because the wave function is compressed along the growth-axis. Therefore excitonic effects become more important than in the bulk semiconductors and excitons may be observed up to room temperature because the thermal ionization is less efficient.[6,7] The same effect as well as an increasing of the oscillator strengths[8] is expected to occur in the case of excitons bound to neutral or ionized impurities. Recombinations due to intentionally introduced defects located in GaAs QW have been studied.[9-12] There are only few theoretical studies concerning bound excitons.[13,14] However, there does not exist, to our knowledge, any theory concerning the exciton-ionized-donor (D^+, X) in QW's, though some transitions identified with this feature have been reported recently.[15] Up to now, only the limit-cases of doped bulk semiconductors,[4] semiconductor surfaces[16] or semi-3D infinite semiconductors[17] have been considered theoretically. In particular, we have shown[16] that the 2D (D^+, X)-energies are about four times greater than those obtained in the 3D case. The energies in the QW are expected to be between the 2D and 3D limits.

In this paper, we report the results of a variational calculation of the energy of the (D^+, X)-complex in a single QW with finite conduction and valence band offsets. We consider a type I semiconductor QW with an ionized donor impurity localized at the centre of the well material that width is L. We suppose that the band offsets are weak enough so that the effective mass approximation may be used. Further, we assume isotropic parabolic non degenerated bands and same electron and hole effective

masses in the well and the barrier materials.

2. GROUND STATE ENERGY AND CONDITION OF STABILITY

The Hamiltonian of an exciton bound to this impurity reads :

$$H = T + V_c + V_w + \epsilon_g \qquad (1)$$

where ϵ_g corresponds to the well material energy-gap discontinuity between conduction and valence bands. T, V_c and V_w denote respectively the kinetic energy operator, the coulombic potential and the total well potential arising from the band offset.

We obtain the ground state energy E and the enveloppe wave function ψ as solutions of the effective Schrödinger equation :

$$(H - \epsilon_g) \psi = E \psi \qquad (2)$$

We choose the following trial wave function[18] :

$$\psi = f_e (z_e) f_h (z_h) (1 + z_e z_h) \exp(-ks/2) \sum_{lmn} C_{lmn} s^l t^m u^n \qquad (3)$$

where z_e and z_h are the electron and hole coordinates along the z-axis which we assume to be parallel to the growth axis. s, t and u define the elliptic coordinates :

$$s = \rho_e + \rho_{eh} \ , \quad t = \rho_e - \rho_{eh} \ , \quad u = \rho_h$$
$$0 \le s \ , \quad -u \le t \le u \ , \quad 0 \le u \le s \qquad (4)$$

where ρ_e , ρ_h and ρ_{eh} are the electron and hole coordinates in the plane perpendicular to the growth axis. l, m, n are positive integers or zero. The linear parameters C_{lmn} as well as the scaling factor k are variational coefficients to be determined by minimizing the mean value of the total energy. The functions f_i (i = e, h) describe the ground states of an electron and a hole in square finite quantum wells of depth V_e and V_h respectively. This wave function, where the in-plane and z-coordinates are separated, is well adapted if the confinement energy is more important than the coulombic energy. In this case, we can replace the coulombic potential by its mean value over the in-plane part of the wave function. In the two limits where L becomes infinity or zero, our wave function becomes questionable because of the separation of the coordinates. However, in the case of infinite well depths and for very small values of L, our function is expected to well describe this 2D-limit.[16]

However, it must be stressed that the observation of the (D^+,X)-complex depends on its stability related to the condition : $E_c \le E_c^D$ or $E \le E^D + E_h$. To verify this inequation it is necessary to know the value of the total energy E_D or the correlation energy $E_c^D = E^D - E_e$ of a neutral donor located at the centre of the well. Therefore we have performed a variational calculation of the correlation energy of donor impurity located at the centre of the well using the following wave function :

$$\psi_D = f_e (z_e) (1 + z_e^2) \exp(- \alpha \rho_e) \qquad (5)$$

where α is a variational parameter.

3. RESULTS AND DISCUSSION

We have calculated the energies E_c as functions of σ, L, V_e, V_h using 34 terms in the developpement of the trial wave function (3). In the present discussion, we apply our results to the case of $GaAs/Ga_{1-x}Al_xAs$. We use the following material data[19] : $m_e / m_0 = 0.0665$ for the electron mass, $m_{hh} / m_0 = 0.34$ and $m_{lh} / m_0 = 0.094$ for the heavy and light holes masses respectively. The band offsets are given by $V_e = Q_e \epsilon_g$ and $V_h = Q_h \epsilon_g$ where $Q_e = 0.57 = 1 - Q_h$. Further we assume that the band gap ϵ_g and the aluminium percentage x are related by[20] : $\epsilon_g = 1.155\ x + 0.37\ x^2$ eV. Using the value[21] $\epsilon = 12.5$

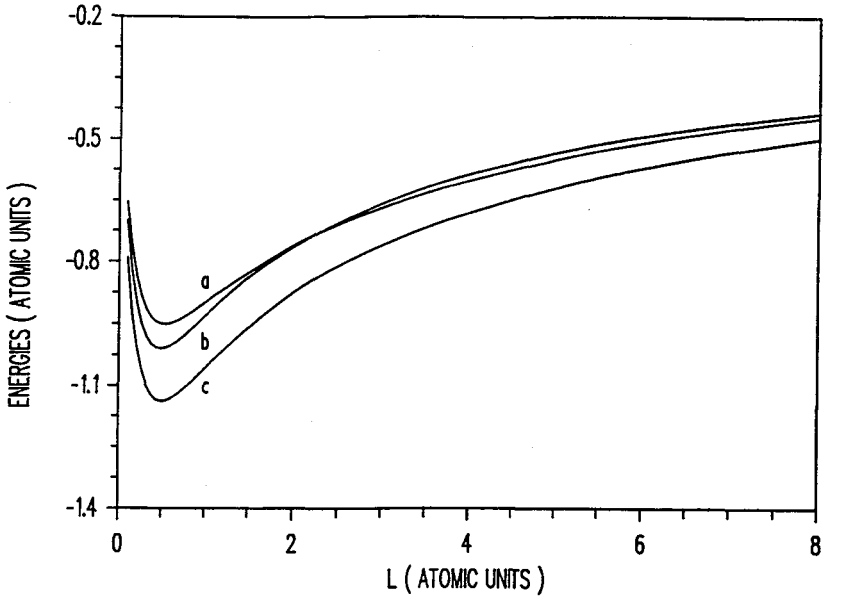

Figure 1 : Variations of the coulombic correlation energy vs. the well width L for a) light (σ = .707) holes, b) donor impurity and c) heavy (σ = .196) holes with x = .15.

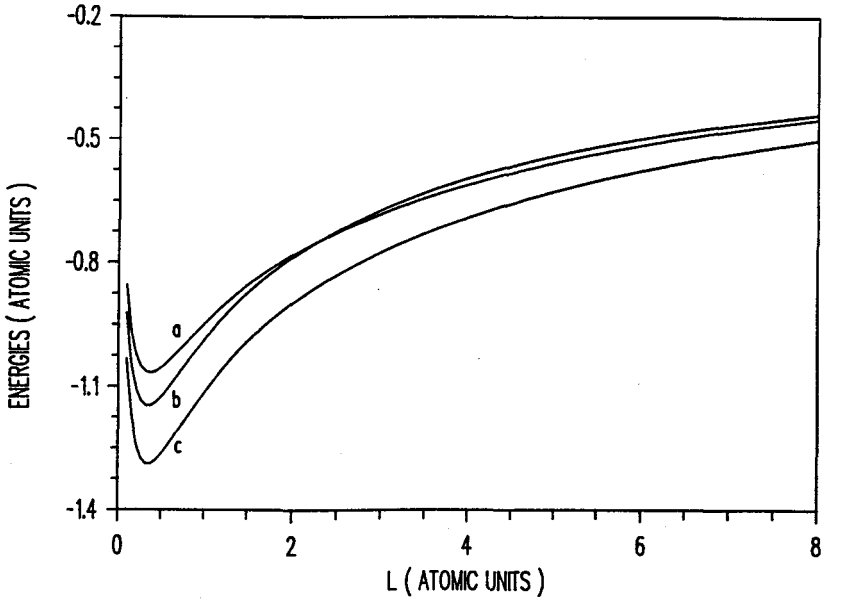

Figure 2 : Variations of the coulombic correlation energy vs. the well width L for a) light (σ = .707) holes, b) donor impurity and c) heavy (σ = .196) holes with x = .30.

for the dielectric constant, we get $a_D = \epsilon\hbar^2/m_e e^2 = 99.5$ Angströms for the effective Bohr radius and $2 R_y = e^2/\epsilon a_D = 11.58$ meV for twice the effective ground state Rydberg of the 3D donor.

Curves a) and c) of Fig. 1 and 2 show the variations of the coulombic correlation energy E_c vs. the well width L for heavy ($\sigma = 0.196$) and light ($\sigma = 0.707$) holes, with x = 0.15 and x = 0.30. All the curves exhibit a pronounced mininimum for $L_m \simeq 50$ Angströms corresponding to a maximum of coulombic binding. In this case we expect the highest oscillator strengths. For $L > L_m$, E_c is an increasing function of L. When L tends to infinity, E_c tends to the 3D-limit[16] corresponding to the given electron to hole effective mass ratio σ whatever the values of x. Nevertheless, our present values are slightly higher than our previous 3D results because our present wave function is not well adapted in this limit. We could improve these results by introducing more terms containing z_e^p or z_h^q in the developpement of the wave function ψ . For $L < L_m$, E_c decreases with L. In this case, the probability of the formation of the (D^+,X)-complex becomes more and more weak due to the fact that the well behaves like a repulsive potential. In the limit where L tends to zero, we get again the 3D E_c values. The same result holds whatever the value of L may be when x tends to zero. Our results may be used to predict the positions of the lines associated with the formation of a (D^+,X)-complex. Indeed the transition energies are given by : $h\nu = \epsilon'_g - E_c$, where $\epsilon'_g = \epsilon_g + E_e + E_h$ is the gap corresponding the the confined particles in the well material. Curves b) of Fig. 1 and 2 show the variations of the donor correlation energies as a function of the well widths L.

Our main result is that the heavy hole ionized bound exciton is stable for all values of L if x = 0.15 and x = 0.30. However, the light hole bound exciton becomes unstable for L < 2.2 at. units and L < 2.1 at. units in the cases where x = 0.15 and x = 0.30 respectively.

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