

## Thomas–Fermi–Dirac calculations of valence band states in two p-type delta-doped ZnSe quantum wells

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We present the hole sub-band structure study in two p-type  $\delta$ -doped ZnSe QW's. An analytical expression for the Hartree–Fock potential is obtained following the lines of the Thomas–Fermi–Dirac (TFD) approximation. We have analyzed the dependence of the hole energy levels to the impurity density and the interlayer distance between wells. The exchange effects are also included in the present survey. We find that many body effects cannot be ignored because these are really important in the calculation at least in the low concentration regime. We have obtained an energy difference between the top of the valence band and the ground energy of the heavy hole ladder of  $E_0 = 29.0$  meV ( $E_g - E_0 = 2.791$  eV) in good agreement with the experimental reports ( $E_{\text{DAP}} = 2.792$  eV) available. We calculate the mobility ratio between double  $\delta$ -doped QW's and simple  $\delta$ -doped QW based on a phenomenological formula. We find the optimum interlayer distance between wells for maximum mobility for three impurity concentrations, which can be of great importance for technological applications.

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### 1 Introduction

With the every day improvement in growth techniques such as MBE and MOCVD has been possible the construction of much more refined systems ( $\delta$ - and modulation-doped systems). The  $\delta$ -doped technique consists in the inclusion of impurities with atomic precision onto some specific semiconductor material. The characterization of  $\delta$ -doped systems (theoretically and experimentally) in III–V compounds (GaAs), Si and more recently in Diamond structures [1–11] is an active field of investigation.

On the other hand, the doping of II–VI semiconductor wide-band-gap materials (ZnSe) [12, 13] is of great importance, due to its possible implementation in blue and green light emitter devices [14, 15], high power THz applications [16], and multiple-wavelength laser diodes [17]. The first highly conductive p-type ZnSe system has been obtained by inserting N-doped ZnTe single monolayers into undoped ZnSe layers [18]. The incorporation of Te, with overall composition of only 9%, and a lattice mismatch as low as 0.6%, effectively enhances the incorporation rate and activity of N. Besides most of the N atoms are in the single  $\delta$ -doped (SDD) ZnTe layers, this avoids the compensation effects commonly observed in highly N-doped ZnSe. The hole concentration is  $7 \times 10^{18}$  cm<sup>-3</sup>, which together with a critical thickness of 500 Å gives a two-dimensional hole charge density  $p_{2D} = 3.5 \times 10^{12}$  cm<sup>-2</sup> for the QW region.

In all  $\delta$ -doped systems the effects of include impurities are: 1) a great amount of carriers is achieved, and 2) several sub-bands are populated. However the localization of the charge distribution near to the ionized impurities leads to a very strong scattering rate as consequence a low mobility. These two parameters are the backbone of the design and manufacture of high power and high velocity semiconductor

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devices. The greatest carrier concentration achievable in a semiconductor system is using the  $\delta$ -doped technique, but the mobility is low ( $10^3 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ) and an improvement is always desirable. One way to improve the mobility is taking into account the coupling of other  $\delta$ -doped layer [4], commonly called double  $\delta$ -doped (DDD) QW's. Due to the interaction between  $\delta$ -doped layers, the average distance between scattering ion centers and the carrier cloud is increased, therefore the dispersion rate goes down and the mobility improvement is obtained. Some works in GaAs and Si report [19–24], an increase of 3 to 5 times respect to a SDD QW's.

In the present paper, the theoretical study of p-type double  $\delta$ -doped ZnSe QW's hole sub-band structure is calculated as a function of the impurity concentration and the interlayer distance between wells. In order to perform our calculations the Thomas–Fermi–Dirac (TFD) approximation is implemented. The TFD theory is the generalization of the Thomas–Fermi (TF) when the many-body effects are considered explicitly in the energy functional. This approximation is known in literature and has been applied to free atoms [25]. In fact, for the case of neutral atoms, it does not lead to any self-consistent solution in which the electron density neither tends to zero at infinity nor indeed to a solution of finite radius in which the boundary density vanishes. Rather, when is used in such a system, there are unavoidable discontinuities in the electron density at the boundary of the atom, which is by all reasons unsatisfactory [25].

If we use the same approximation to describe the conduction band bending of a semiconductor caused by an electric charge in some region of space, exactly the same problem would occur. However, when the TFD approximation is applied to p-type systems (holes), this leads to a self-consistent and physically meaningful solution [26], in contrast to n-type systems [25]. Keeping in mind all these details, it is possible to obtain an analytical expression for the Hartree–Fock potential within the formal structure of the TFD approximation. Such expression is used to solve two or three uncoupled Schrödinger like-equations one for each hole ladder: heavy hole (hh), light hole (lh) and split-off (so) one. What determines the use of two or three bands (the inclusion of the so band)? To answer this question it is necessary to attend the main features and the backbone parameters that play a fundamental role in our system. First of all, the relative energy alignment of the so band respect to the Brillouin zone center may change drastically depending of the concrete host material used. The other fundamental factor is the impurity concentration because the potential depth depends directly on this factor. As the impurity density increases the potential well depth also does. Then at least in the high impurity regime the so band could take relevance, since it is possible to bound so states (as has been demonstrated for GaAs and Si systems [27, 28]). In this work we ignore the influence of the so band, due to the energy distance between the hh band and the lh band to the so band (430 meV), and as the calculation is restricted only to the physically meaningful impurity density interval, in which the potential well depth never exceeds the so energy distance to the zone center. We solve numerically two uncoupled Schrödinger like-equations in order to obtain the corresponding hole ladder.

Based on the hole level structure and the wave functions, we study the transport properties of our system. A phenomenological formula for the mobility ratio between DDD QW's and SDD QW is implemented. In this study only the most important scattering mechanism at low temperature is considered, i.e., the ionized impurities.

The paper is arranged as follows: in the next section the method and model is presented, following with the results and analysis, and finally the conclusions are given.

## 2 Mathematical method

The TFD energy functional ( $E_{\text{TFD}}$ ) must be constructed. Here and henceforth we assume to be in the low temperature limit. Therefore the kinetic energy can be written as [25]

$$t = \frac{3 \left[ 3\pi^2 \hbar^3 p(r) \right]^{2/3}}{10 m_{\text{hh}} m_a} \quad (1)$$

with  $m_a = \left[ 1 + \left( \frac{m_{lh}}{m_{hh}} \right)^{3/2} \right]^{2/3}$ , where  $m_{hh}$  and  $m_{lh}$  are the heavy and light hole masses respectively. The kinetic energy functional is

$$T = \int p(r) t \, dr = \frac{3}{10m_{hh}m_a} \int p(z) [3\pi^2 \hbar^3 p(z)]^{2/3} dz. \quad (2)$$

The energy functional of the hole–hole interaction is

$$V_{hh} = \frac{e^2}{2\epsilon_r} \iint \frac{p(r) p(r')}{|\mathbf{r} - \mathbf{r}'|} \, dr \, dr' \quad (3)$$

then going over polar coordinates and neglecting the self-interaction energy

$$V_{hh} = -\frac{e^2 \pi}{\epsilon_r} \iint p(z) p(z') |z - z'| \, dz \, dz'. \quad (4)$$

This last equation is very interesting, since, the self-energy is omitted and is expected that our calculations would be closer to the experimental measurements. The other interesting feature is the negative sign, in contradiction with the logical sense of a repulsion interaction. This characteristic is also presented in electronic systems [30].

The interaction between the hole gas and the two impurity planes is described by the following density functional:

$$V_{hh} = \int p(r) V_N(r) \, dr = \frac{2e^2 \pi}{\epsilon_r} (p_{2D}^1 \int p(z) |z + l/2| \, dz + p_{2D}^2 \int p(z) |z - l/2| \, dz). \quad (5)$$

Here,  $p_{2D}^1$  and  $p_{2D}^2$  are the impurity spikes in well 1 and 2, and  $l$  is the interlayer distance between the wells. Finally the exchange energy for a hole gas with valence band coupling is [31, 32]

$$\epsilon_x(r) = -\zeta(w) \frac{3a_0^*}{2\pi} (3\pi^2 p(r))^{1/3} R_y^* \quad (6)$$

where

$$\zeta(w) = 2^{-1/3} + (1 - w^2) [w^2 (aw + b) + c(4w^3 + 3w^2 + 2w + 1)] \quad (7)$$

with  $w = \frac{m_{lh}}{m_{hh}}$ ,  $a = 0.679$ ,  $b = -0.0686$ , and  $c = -0.0811$ . The factor  $\zeta(w)$  is always smaller when we consider uncoupled bands, in which case  $\zeta(w) = (1 + w^4)/(1 + w^3)^{4/3}$  [32]. At this point as the problem is not much more complicated we will use the expression (7) for the parameter  $\zeta(w)$  considering coupled bands. The exchange energy functional is

$$E_x = \int p(r) \epsilon_x(p(r)) \, dr \quad (8)$$

substituting (6) in (8)

$$E_x = -\zeta(w) \frac{3a_0^*}{2\pi} R_y^* \int p(z) (3\pi^2 p(z))^{1/3} \, dz. \quad (9)$$

The total TFD density functional is given of the following way

$$\begin{aligned} E_{TFD} = & \frac{3}{10m_{hh}m_a} \int p(z) [3\pi^2 \hbar^3 p(z)]^{2/3} dz - \frac{e^2 \pi}{\epsilon_r} \iint p(z) p(z') |z - z'| \, dz \, dz' \\ & + \frac{2e^2 \pi}{\epsilon_r} (p_{2D}^1 \int p(z) |z + l/2| \, dz + p_{2D}^2 \int p(z) |z - l/2| \, dz) - \frac{3a_0^* \zeta(w) R_y^*}{2\pi} \\ & \times \int p(z) (3\pi^2 p(z))^{1/3} \, dz. \end{aligned} \quad (10)$$

It is well known that if we apply the variational principle  $\delta(E_{\text{TFD}} - \mu N) = 0$  and calculate it by standard procedure we find the Lagrange multiplier  $\mu$  identifying it as the chemical potential. If we consider the effective units  $R_y^* = e^2/(2\varepsilon_r a_0^*)$  and  $a_0^* = \varepsilon_r \hbar^2/(e^2 m_{\text{nh}})$ . Defining  $p_{\text{au}}(z) = (a_0^*)^3 p(z)$  it is possible to write the chemical potential as:

$$\begin{aligned} \mu = & \frac{1}{m_a} \left[ 3\pi^2 p_{\text{au}}(z) \right]^{2/3} - \frac{2e^2 \pi}{\varepsilon_r} \int p(z) |z - z'| dz \\ & + \frac{2\pi e^2}{\varepsilon_r} (p_{2D}^1 |z + l/2| + p_{2D}^2 |z - l/2|) - \zeta(w) \frac{2}{\pi} (3\pi^2 p_{\text{au}}(z))^{1/3} R_y^* . \end{aligned} \quad (11)$$

On the other hand, the spatial band bending is described by the Poisson equation:

$$\frac{d^2 V_H(z)}{dz^2} = -\frac{4\pi e^2}{\varepsilon_r} p(z) + \frac{4\pi e^2}{\varepsilon_r} \{ p_{2D}^1 \delta(z + l/2) + p_{2D}^2 \delta(z - l/2) \} \quad (12)$$

and

$$V_H(z) = -\frac{2e^2 \pi}{\varepsilon_r} \int p(z) |z - z'| dz + \frac{2\pi e^2}{\varepsilon_r} (p_{2D}^1 |z + l/2| + p_{2D}^2 |z - l/2|) \quad (13)$$

where  $V_H(z)$  is the well known Hartree potential. Taking into account (13), the chemical potential (11) is

$$\mu = \left[ \frac{3\pi^2 p_{\text{au}}(z)}{m_a^{3/2}} \right]^{2/3} R_y^* + V_H(z) - \frac{2\zeta(w)}{\pi} (3\pi^2 p_{\text{au}}(z))^{1/3} R_y^* \quad (14)$$

Solving the quadratic equation for  $p_{\text{au}}(z)$  in (14) and remaining with the physically meaningful solution

$$p_{\text{au}}(z) = \frac{m_a^3 \zeta^3(w)}{3\pi^5} \left[ 1 - \sqrt{1 + \frac{\pi^2 (\mu^* - V_H^*(z))}{\zeta^2(w) m_a}} \right]^3 \quad (15)$$

where  $V_H^* = V_H/R_y^*$  and  $\mu^* = \mu/R_y^*$ . Replacing  $p_{\text{au}}(z)$  in the Poisson equation,

$$\frac{d^2 V_H^*(z)}{dz^2} = -\frac{8m_a^3 \zeta^3(w)}{3\pi^4} \left[ 1 - \sqrt{1 + \frac{\pi^2 (\mu^* - V_H^*(z))}{\zeta^2(w) m_a}} \right]^3 + 8\pi p_{2D}^1 \delta(z + l/2) + 8\pi p_{2D}^2 \delta(z - l/2) \quad (16)$$

the solution to this equation would provide a Hartree–Fock self-consistent solution. Since Eq. (26) is a non-linear one, its solution is not trivial. It must always be carried out numerically; in which case, it should be no more convenient than carrying out a self-consistent calculation. Then in order for our method to be advantageous, we carried out an additional approximation. The many-body effects alters the hole sub-band structure in the following way; first of all the exchange effects through the exchange potential in the Schrödinger equation generates a change in the valence band states. Therefore, this change in the hole sub-band structure modifies the charge density; hence as a consequence the Hartree potential would be modified. Let us suppose that the presence of exchange practically unchange the Hartree potential, i.e. we are supposing that the presence of exchange alters the level structure and the charge density, but we discard change in the form of the Hartree potential by the presence of exchange, all of this within a quasi-classical approximation. In such a case the corresponding Poisson equation (in effective units) that must be solved is

$$\frac{d^2 V_H^*(z)}{dz^2} = -\frac{8m_a^{3/2}}{3\pi} (\mu^* - V_H^*(z))^{3/2} + 8\pi \{ p_{2D}^1 \delta(z + l/2) + p_{2D}^2 \delta(z - l/2) \} . \quad (17)$$

If the impurity concentration is the same in both wells ( $p_{2D}^1 = p_{2D}^2 = p_{2D}$ ), the system is symmetric with respect to the central point, so, the Hartree potential is an even function and we can work with only one side ( $z \leq 0$ ).

$$\frac{d^2 V_H^*(z)}{dz^2} = -\frac{8m_a^{3/2}}{3\pi} (\mu^* - V_H^*(z))^{3/2} + 8\pi p_{2D} \delta(z+l/2) \quad (18)$$

the specific and physically meaningful solution of this type of equation as is stated by Ioriatti [33] is of the form  $1/f^4(z)$ , where  $f(z)$  is a linear function of  $z$ . In the case of double  $\delta$ -doped QW's the solution is

$$V_H^*(z) - \mu^* = -\frac{\alpha^2}{(\alpha|z+l/2|+z_0)^4} \quad (19)$$

substituting this into (18) we find  $\alpha$ ,

$$\alpha = \frac{2m_a^{3/2}}{15\pi} \quad (20)$$

and the neutrality charge requirement gives

$$z_0 = \left( \frac{\alpha^3}{\pi p_{2D}} \right)^{1/5}. \quad (21)$$

Substituting (19) in (15), the charge density is

$$p_{au}(z) = \frac{m_a^3 \zeta^3(w)}{3\pi^5} \left[ 1 - \sqrt{1 + \frac{\pi^2}{\zeta^2(w) m_a} \frac{\alpha^2}{(\alpha|z+l/2|+z_0)^4}} \right]^3. \quad (22)$$

At this point we use an expression obtained within the Local Density Approximation (LDA) [36] for the exchange potential,

$$V_x^*(z) = -\zeta(w) \frac{2}{\pi} (3\pi^2)^{1/3} (p_{au}(z))^{1/3} \quad (23)$$

substituting (22) in (23), we obtain

$$V_x^*(z) = -\frac{2\zeta^2(w) m_a}{\pi^2} \left[ 1 - \sqrt{1 + \frac{\pi^2}{\zeta^2(w) m_a} \frac{\alpha^2}{(\alpha|z+l/2|+z_0)^4}} \right] \quad (24)$$

At low temperatures, the Fermi level is located only very few meV above the bands' edge [34, 35]. Therefore is a good approximation to take it coinciding with the potential well vertex. Finally the total potential,  $V^*(z) = V_H^*(z) + V_x^*(z)$ , is

$$V^*(z) = -\frac{\alpha^2}{(\alpha|z+l/2|+z_0)^4} - \frac{2\zeta^2(w) m_a}{\pi^2} \left[ 1 - \sqrt{1 + \frac{\pi^2}{\zeta^2(w) m_a} \frac{\alpha^2}{(\alpha|z+l/2|+z_0)^4}} \right]. \quad (25)$$

The last equation summarizes the model for the total potential of p-type DDD ZnSe QW's. Such equation is substituted into two uncoupled Schrödinger like equations in order to obtain the heavy and light hole ladders. In this way we can avoid a troublesome and long self-consistent calculation.

Besides this method allows us to study the transport properties of the system. We only consider the ionized acceptor scattering mechanism because it is the most important at low temperature. The Cou-

lomb scattering potential due to ionized impurities is considered as distributed randomly in the doped layer. We take the ratio of the mobility of DDD to SDD QW's [3].

$$\mu_{\text{rel}}^{\delta} = \frac{\mu_{\text{DDD}}}{\mu_{\text{SDD}}} = \frac{\sum_j m_j^* \sum_i \int |F_e^{\delta}(z')|^2 (k_F^{\delta} - E_i^{\delta}) |z'| dz'}{\sum_j m_j^* \sum_i \int |F_e^{2\delta}(z')|^2 (k_F^{2\delta} - E_i^{2\delta}) (|z' - l/2| + |z' + l/2|) dz'} \quad (26)$$

where  $F_e^{\delta}(z')$ ,  $k_F^{\delta}$  and  $E_i^{\delta}$  ( $F_e^{2\delta}(z')$ ,  $k_F^{2\delta}$  and  $E_i^{2\delta}$ ) are the envelope function, the Fermi level and the  $i$ th level respectively of the SDD (of DDD).

In [37] has been calculated the influence of the temperature to the electronic structure. The results have shown a slightly modification of the level structure when the temperature is less than 6 meV (77 K). In such a case the electronic structure can be taken as that corresponding to 0 K and the thermal effect can be considered as a charge redistribution. Then, the mobility expression would be

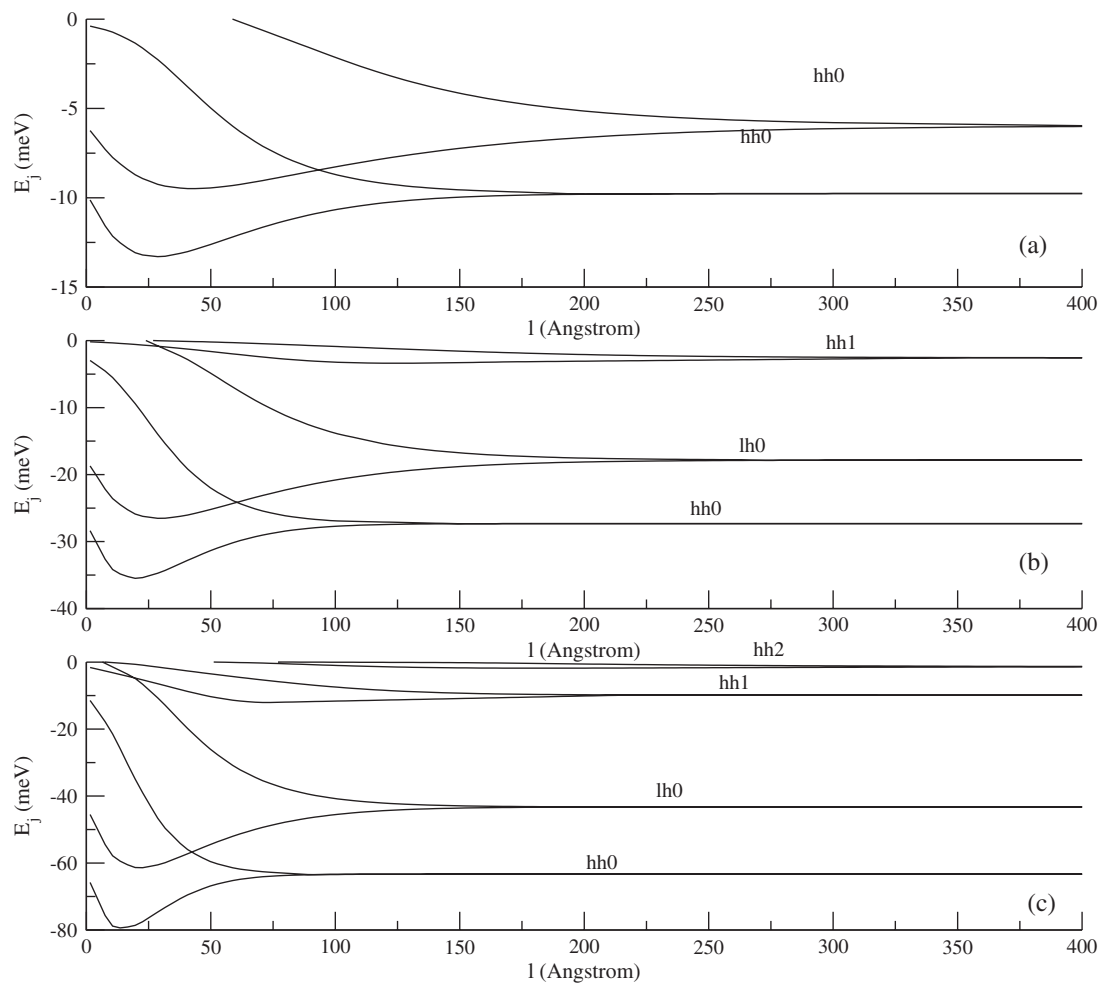
$$\mu_{\text{rel}}^{\delta} = \frac{\sum_j m_j^* \sum_i \int |F_e^{\delta}(z')|^2 \ln \left[ 1 + e^{(k_F^{\delta} - E_i^{\delta})/k_B T} \right] |z'| dz'}{\sum_j m_j^* \sum_i \int |F_e^{2\delta}(z')|^2 \ln \left[ 1 + e^{(k_F^{2\delta} - E_i^{2\delta})/k_B T} \right] (|z' - l/2| + |z' + l/2|) dz'} \quad (27)$$

### 3 Results and discussion

The starting parameters for ZnSe are the typical standard ones:  $E_g = 2.82$  eV,  $\epsilon(0) = 8.7$ ,  $\epsilon(\infty) = 5.8$ ,  $m_{\text{nh}} = 0.49$ , and  $m_{\text{h}} = 0.15$ . We consider three different impurity concentrations  $1 \times 10^{12} \text{ cm}^{-2}$  (a),  $3.5 \times 10^{12} \text{ cm}^{-2}$  (b) and  $1 \times 10^{13} \text{ cm}^{-2}$  (c). In Fig. 1 we show the dependency of the hole sub-band structure versus the distance between the impurity planes for the impurity concentrations (a), (b) and (c), the exchange effects have been considered. Figure 1 reveals that by increasing the impurity plane distance, the hole energy levels are degenerated, depending on what level we are considering. On the other hand, increasing the impurity concentration, the hole energy levels degenerate at a lesser interlayer distance and other hole levels could be trapped, since the potential depth increase as well.

In fact, the same effect is introduced when we consider the many-body interaction (Fig. 2). In that figure we sketch the potential profile and the heavy and light hole wave functions for the different hole energy levels. Figure 2(a) and (b) are omitting and taking into account the exchange effects for the same impurity concentration. The symmetry requirements are well fulfilled.

Another important feature, specific of the DDD QW's is that given an impurity concentration (into the physically meaningful range), we will have a specific heavy and light hole ladders. These hole energy levels of the two coupled delta-doped QW's behave like (as a function of the impurity plane distance) if we have a SDD QW, with the only difference that the SDD QW is wider, so, the energy levels go down as the distance between impurities planes increases. However this behavior stops at certain distance depending what hole level we are taking into account, because energetically the hole levels are very different as well as the barrier penetration is. Then when this happens the DDD QW behavior takes place; the energy levels go up until the degeneration occurs, recovering the SDD QW and their hole sub-band structure as a consequence. This resembles the typical molecular formation curves. At  $l = 0$  the same thing happens, the energy level structure corresponds to an SDD QW. Therefore the hole sub-band structure is the same when no barrier exists ( $l = 0$ ) and when the barrier is infinite. Here, there is a great difference with respect to a rectangular QW, because when no barrier exists in a rectangular potential profile, the QW width is larger, exactly the double, if both wells have the same size. Then, in this case, the energy level structure is very different depending on the existence (or nonexistence) of quantum barriers.

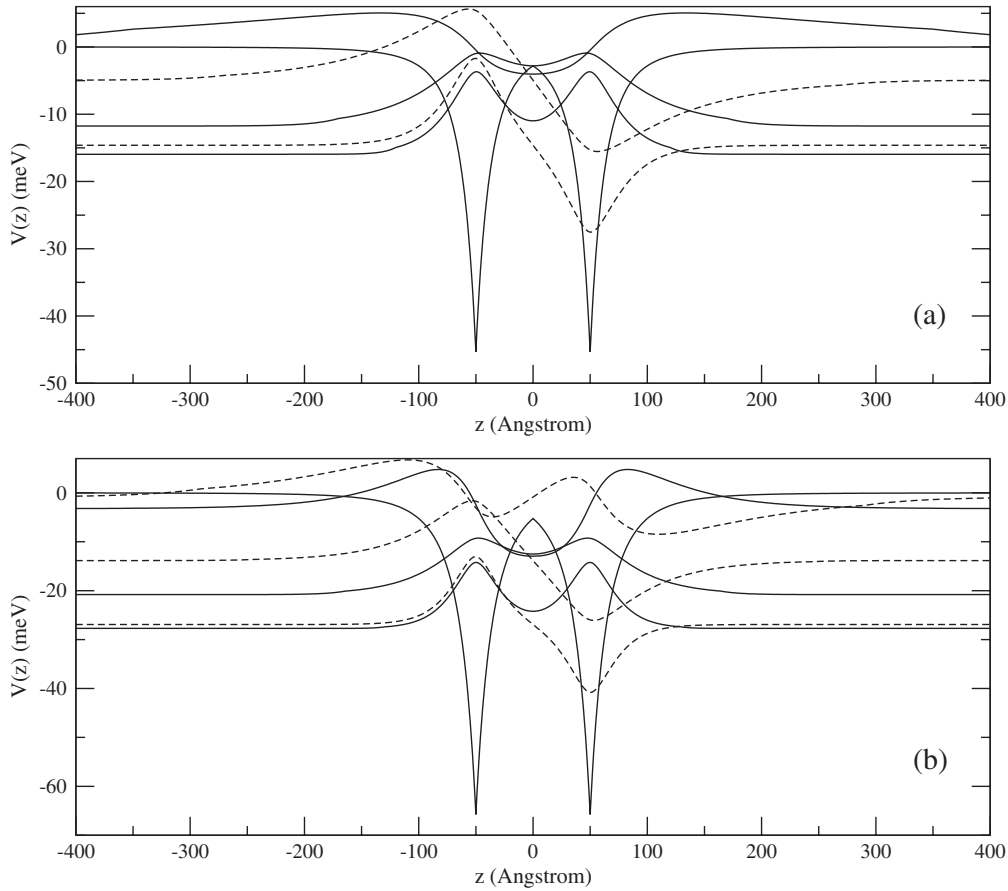


**Fig. 1** Hole levels versus the interlayer distance between wells for:  $1 \times 10^{12} \text{ cm}^{-2}$  (a),  $3.5 \times 10^{12} \text{ cm}^{-2}$  (b) and  $1 \times 10^{13} \text{ cm}^{-2}$  (c), taking into account the many-body effects.

In Table 1 a summary of the paramount features of the system is presented, for the impurity concentration range of interest. Features: degeneracy distance, potential depth, degeneracy energy difference between ground and first excited heavy hole states ( $E_{\text{hh}0} - E_{\text{hh}1}$ ), and between ground heavy and ground light hole states ( $E_{\text{hh}0} - E_{\text{lh}0}$ ), taking into account the exchange effects (ex) and without them (wex).

We can see from the table that many body effects are of considerable importance in the low concentration regime, because, for an impurity density of  $1 \times 10^{12} \text{ cm}^{-2}$  the difference between degeneracy distances omitting and taking into account the many body effects is about  $70 \text{ \AA}$  for the heavy hole ground state, while for an impurity density of  $1 \times 10^{13} \text{ cm}^{-2}$  it is about  $10 \text{ \AA}$ .

Our numerical results give the value  $E_0 = 29.0 \text{ meV}$  ( $l=0$ ) for the energy difference between the top of the valence band and the  $\Gamma$ -point of the Brillouin zone and the quantized level corresponding to the heavy hole ladder,  $E_{\text{hh}0}$ . The two dimensional hole concentration in the quantum well used in the evaluation is  $p_{2\text{D}} = 3.5 \times 10^{12} \text{ cm}^{-2}$ . Our  $E_0$  ( $l=0$ ) agrees very well with the hole activation energy estimated by Jung [18] for the same sample, from the slope of the hole concentration versus the inverse of the temperature at low temperatures  $E_a = 30 \text{ meV}$ . This constitutes a reduction of  $E_a$  from the reported acceptor binding energy in ZnTe [38], which had already been observed in bulk ZnSe:N [39]. According to what has been discussed in the present work, this smaller value would arise as a conse-



**Fig. 2** Potential profile and hole wave functions for  $p_{2D} = 3.5 \times 10^{12} \text{ cm}^{-2}$  omitting (a) and taking into account (b) the many-body effects. The solid (dashes) lines correspond to the even (odd) heavy and light hole levels.

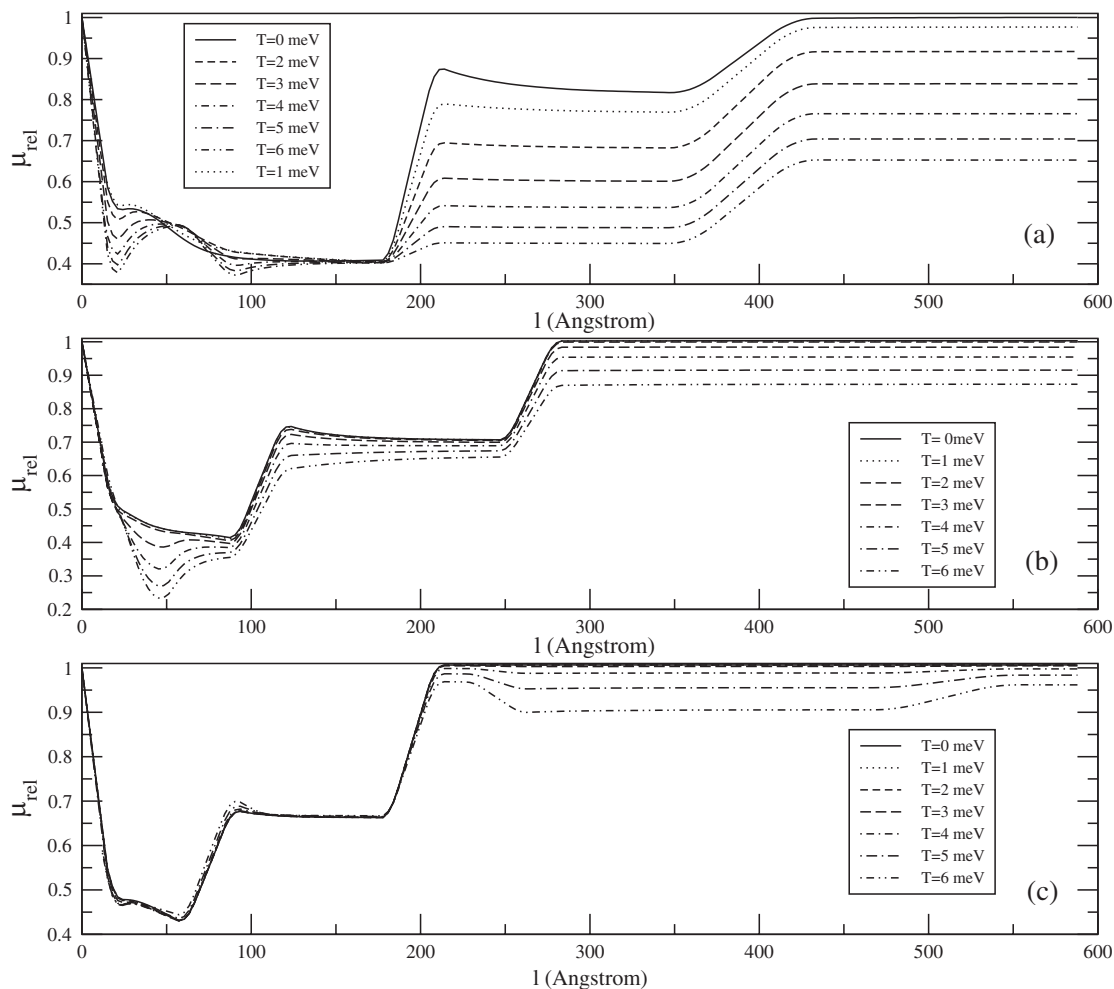
quence of many-body effects, which we introduce in the single particle states through the Hartree–Fock potential derived from TFD considerations, but supporting the conjecture of Fan et. al. [39].

Additionally, this result for  $E_0$  ( $l = 0$ ) is in close agreement with the energy of the transition between the shallow and the acceptor pair reported by Han [38] for the dominant acceptor bound exciton emission in the photoluminescence spectrum of the ZnSe/ZnTe:N delta-doped layer structure with the same

**Table 1** Paramount features of DDD ZnSe QW's: degeneracy distance for heavy, light, and first excited heavy hole levels (hh0, lh0, hh1), potential depth, and the degeneracy energy difference  $E_{hh0} - E_{hh1}$  and  $E_{hh0} - E_{lh0}$ , with (ex) and without (wex) exchange effects.

$p_{2D}$ ( $10^{12} \text{ cm}^{-2}$ )		degeneracy distance			potential depth (meV)	$E_{hh0} - E_{hh1}$ (meV)	$E_{hh0} - E_{lh0}$ (meV)
		hh0	lh0	hh1			
1	wex	300	500		-16.633		-2.083
	ex	220	380		-26.936		-3.792
3.5	wex	170	320		-45.314		-06.209
	ex	140	250	350	-65.743	-24.746	-09.480
10	wex	100	200	320	-104.950	-38.403	-15.001
	ex	90	170	220	-139.347	-53.468	-20.083





**Fig. 3** Mobility calculations for  $p_{2D} = 1 \times 10^{12} \text{ cm}^{-2}$  (a),  $3.5 \times 10^{12} \text{ cm}^{-2}$  (b) and  $1 \times 10^{13} \text{ cm}^{-2}$  (c). The solid, dot, dashed, etc. curves, correspond to the different temperatures in the range of 0–7 meV in each case (the temperature is augmented 1 meV gradually).

$p_{2D}$ :  $E_{DAP} = 2.792 \text{ eV}$ . The numerical value of this quantity, arising from the present model is  $E_g - E_0 = 2.791 \text{ eV}$  ( $l = 0$ ). It is worth mentioning that recent reports on this class of systems seem to be in contradiction with the value  $E_{DAP}$  used here. The positions of low temperature photoluminescence peaks observed in such work [40] for a SDD well are about 100 meV below this transition energy, which is attributed there to the diffusion of N atoms from the ZnSe:N buffer layer. However, it is not possible for us to calculate hole levels for this latter case due to the lack of accurate information concerning the values of the hole concentration in their samples. The main drawback in this subject is the absence of additional experimental reports about ZnSe/ZnTe:N delta-doped samples with values of  $p_{2D}$  over a wider range of hole densities. Nonetheless, our numerical outputs ( $l = 0$ ) are in good agreement with the experimental ones, at least for the only experimental data available for comparison. Also it is important to remark that this close agreement among us and the experimental colleagues could be possible because we are omitting the self-interaction energy in our calculations, as we can see in the formal development of TFD approximation.

In Fig. 3 the mobility calculation are presented for three impurity concentrations. The temperature dependence is also analyzed in the range of 0–7 meV. In Fig. 3(a) a main peak is found around 210 Å

and as soon as the temperature increases a second peak appears at 50 Å. An augmentation of the impurity density comes with a shift of the main peak to 120 Å as well as a minimum in the mobility at 45 Å is presented. In the high density limit (Fig. 3(c)) the paramount peak is around 90 Å and when the temperature increases a second peak appears at 220 Å. Finally when the interlayer distance is long enough in such a way that the inter-well interaction practically vanishes the mobility ratio tends to one.

## 4 Conclusions

In summary, we have studied the hole sub-band structure of DDD ZnSe QW's as a function of the main parameters in the system: impurity density, interlayer distance between the wells and the exchange effects. In order to accomplish such study the TFD approximation has been applied. An analytical expression for the Hartree–Fock potential is obtained. This equation allows us to avoid a troublesome and long self-consistent procedure and treat the many-body effects as well. The hole sub-band structure study shows that exchange effects are more important in the low concentration regime, therefore if we omit these in the calculation, a gross error would be committed. Also a close agreement is obtained with respect to the experimental data, due on one hand to the inclusion of many-body effects, and on the other to the elimination of the self-energy in our calculations, as is demonstrated in the formal development of the TFD approximation.

The phenomenological formula for the mobility ratio between DDD QW's and SDD QW permits us to obtain the trends of this important quantity. We find the optimum interlayer distance between wells and impurity density to achieve the maximum mobility.

Although, in spite of the scarce experimental information which is the main inconvenient in this subject, the TFD approximation, even though it is simple, it shows that is a useful tool and gives accurate results. The hole sub-band structure calculation reveals the main features of the double DDD ZnSe QW's. It also allows us to determine the importance of many-body effects onto the system as well as find the optimum interwell distance and impurity density to obtain the maximum mobility.

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