ELECTRIC FIELD EFFECTS ON THE EXCITON BOUND TO AN IONIZED DONOR IN PARABOLIC QUANTUM WELLS

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Using a perturbation-variational procedure within the effective-mass approximation we investigate the ground-state properties of an exciton bound to an ionized donor in a parabolic quantum well under the action of the electric field. We used a screened potential for the hole-ionized donor interaction and we calculated the binding energy as a function of the electric field, the donor-impurity position and the screening parameter. We found that the presence of the electric field breaks down the degeneracy of states for the impurities symmetrically positioned in the well, and together with the screened potential effect is determinant for the existence of bound states in these structures.

1. Introduction

Stimulated by the rapid progress in nanometer-scale fabrication technology, a large number of papers focused on the optical properties of low-dimensional systems has been published. As in 3D semiconductors, optical excitations may give rise to "exciton" (X) or "bound-exciton" (BE) states. The three particle complex (D^+, X) consisting of an electron and a hole bound to an ionized donor is the simplest possible bound-exciton complex. Their possible existence in semiconductors was proved theoretically in 1958 by Lampert [1]. As in 3D semiconductors the binding energies of BE complexes are generally low, their stability has been the subject of several theoretical studies. As a result, it appears [2] that the (D^+, X) complex is only stable if the elctron to hole effective mass ratio $\sigma = m_e / m_h$ is less than the critical value $\sigma_c = 0.454$.

Recently, there has been a great interest in the study of excitons bound to an ion in confined geometries, such as quantum wells, wires and dots [3-11]. In lower dimensions, because the overlapping between the wave functions of the electron and the hole becomes more important, the exciton and BE states are more bound than in the bulk. Moreover, if the confinement potentials may be modeled by an infinitely deep potential well, the possible stability problem no longer occurs because, in this case, all the particles remain confined in a finite space. So it is expected that the observation of bound excitons should be more easy in these structures than in 3D semiconductors. The variational determination of the ground-state energies of the (D^+, X) complex in two-dimensional semiconductors and semiconductor quantum wells has been presented in [6-9]. The effect of the quantum confinement on the electronic and optical properties of an exciton bound to an ionised hydrogenic donor placed at the center of a semiconductor spherical microcrystal has been studied in [8]. The dependence of the binding energies of (D^+, X) complex in a two-dimensional quantum dot has been obtained as a function of the electron-to-hole mass ratio [10]. Total energy, binding energy, recombination rate for an exciton bound in a two-dimensional quantum dot by a donor impurity have been calculated by using the Hartree formalism in Ref. [11].

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However, up to now, there are no theoretical reports about the effects of applied electric fields on the binding energy of an exciton bound to a charged impurity in parabolic quantum wells. In this paper we present a perturbation-variational determination of the ground-state energy of the (D^+, X) complex with a hydrogenic donor impurity in a parabolic quantum well (PQW) under an electric field.

2. Theory

Within the effective-mass approximation and assuming isotropic, parabolic and nondegenerated bands, the Hamiltonian of the (D^+, X) complex in a PQW can be written as:

$$H = H_z^e + H_z^h + \frac{1}{2\mu}(p_x^2 + p_y^2) - \frac{e^2}{\sqrt{\rho_{eh}^2 + (z_e - z_h)^2}} + V_c^e(\vec{r}_e) + V_c^h(\vec{r}_h) \qquad (1)$$

Here

$$H_z^e = \frac{(p_z^e)^2}{2m_e} + V_w^e + |e|F z_e \qquad (2a)$$

and

$$H_z^h = \frac{(p_z^h)^2}{2m_h} + V_w^h - |e|F z_h \qquad (2b)$$

are the Hamiltonians describing the z confinement of the electron and hole in a PQW under an electric field perpendicular to the well interfaces. μ is the reduced effective mass in the well plane and $\vec{\rho}_{eh} = \vec{\rho}_e - \vec{\rho}_h$, were ρ_i $(i = e, h)$ denote the position in-plane for each particle. V_w^i are the electron and hole PQW potentials with the well width L:

$$V_w^i = \begin{cases} \dfrac{k_i z_i^2}{2}; & |z_i| \leq \dfrac{L}{2} \\ V_i; & |z_i| > \dfrac{L}{2} \end{cases} \qquad (3)$$

where V_e and V_h are the electron and hole band offsets.

Under the assumption that the exciton binding is only a weak perturbation to the total energy, which is satisfied for not too narrow wells, we can first solve the Equations (2) which give us the electron and hole PQW ground state wave functions, $\Phi_e(z_e)$ and $\Phi_h(z_h)$, respectively, with the corresponding energies E_e and E_h.

It has been proved [8,13] that for the excitons in GaAs–Al$_x$Ga$_{1-x}$As low-dimensional systems, as the hole is a rather heavy particle and the valence band confining potential is quite small, the hole spatial extension $<r_h>$ is larger than the electron extension $<r_e>$. The effect is more pronounced when an electric field is applied due to the stronger polarization of the hole. Therefore, a more realistic potential for the interaction between the hole and the donor impurity, which takes into account the spread of the hole wave function, is the Debye (or screened Coulomb) potential [15,16]:

$$V_c^h = \frac{e^2 \exp(-\beta r)}{\varepsilon r} \qquad (4)$$

where β is the screening parameter. For the interaction between the electron and the impurity we choose a no screened Coulomb potential. Thus interaction between the carriers and the impurity located at $(0, 0, z_i)$ is given by:

$$V_c^e = -\frac{e^2}{\varepsilon\sqrt{\rho_e^2 + (z_e - z_i)^2}} \tag{5a}$$

$$V_c^h = \frac{e^2 \exp\left(-\beta\sqrt{\rho_h^2 + (z_h - z_i)^2}\right)}{\varepsilon\sqrt{\rho_h^2 + (z_h - z_i)^2}} \tag{5b}$$

In the narrow parabolic well and for small electric field, the quantum confinement are much stronger than electron (hole)-impurity interaction. Therefore in the perturbation-variational method that is proposed here, the Hamiltonian (1) is rewritten as

$$H = H_0 + H_p \tag{6}$$

with the perturbing term

$$H_p = V_c^e + V_c^h \tag{7}$$

We solved the unperturbed Hamiltonian H_0 using the variational principle with the separate trial functions

$$\psi_{nl}(\rho_{eh}, z_e, z_h) = \phi_e(z_e)\,\phi_h(z_h)\,\chi_{nl}(\rho_{eh}) \tag{8}$$

where $\chi_{nl}(\rho_{eh})$ are 2D hydrogenic functions which describe the bound states of the electron-hole relative motion [17]. For the ground state of exciton

$$\chi_{1s} = \exp\left(-\rho_{eh}/\lambda\right) \tag{9}$$

Here λ is a variational parameter determined by minimizing the exciton energy:

$$E_{ex} = \min_{\lambda}\left(\frac{\langle\psi_{1s}|H_0|\psi_{1s}\rangle}{\langle\psi_{1s}|\psi_{1s}\rangle}\right). \tag{10}$$

The first-order correction for the ground-state of the exciton complex due to the perturbing Hamiltonian H_p is:

$$E^{(1)} = \frac{\langle\psi_{1s}|H_p|\psi_{1s}\rangle}{\langle\psi_{1s}|\psi_{1s}\rangle} \tag{11}$$

The total energy of the $\left(D^+, X\right)$ complex is given by:

$$E\left(D^+, X\right) = E_{ex} + E^{(1)} \tag{12}$$

and the binding energy is defined as [18]:

$$E_b = E\left(D^0\right) + E_h - E\left(D^+, X\right). \tag{13}$$

where $E\left(D^0\right)$ is the ground-state energy of the neutral donor in the well.

3. Results and discussion

We have calculated the ground-state energy of the exciton complex as a function of the electric applied field and for various impurity distances z_i from the QW center. The numerical solutions discussed here were obtained for a GaAs-$Al_{0.32}Ga_{0.68}As$ parabolic quantum well with $L = 10$ nm, where we took as material parameters $\varepsilon = 12.4$, $m_e = 0.067\,m_0$, $\sigma = 0.707$, $V_e = 244\,meV$ and $V_h = 163\,meV$. Also we use the effective screening parameter $\alpha = \beta\,a*$, where $a*$ is the effective Bohr radius $a* = \dfrac{\hbar^2\varepsilon}{m_e\,e^2}$.

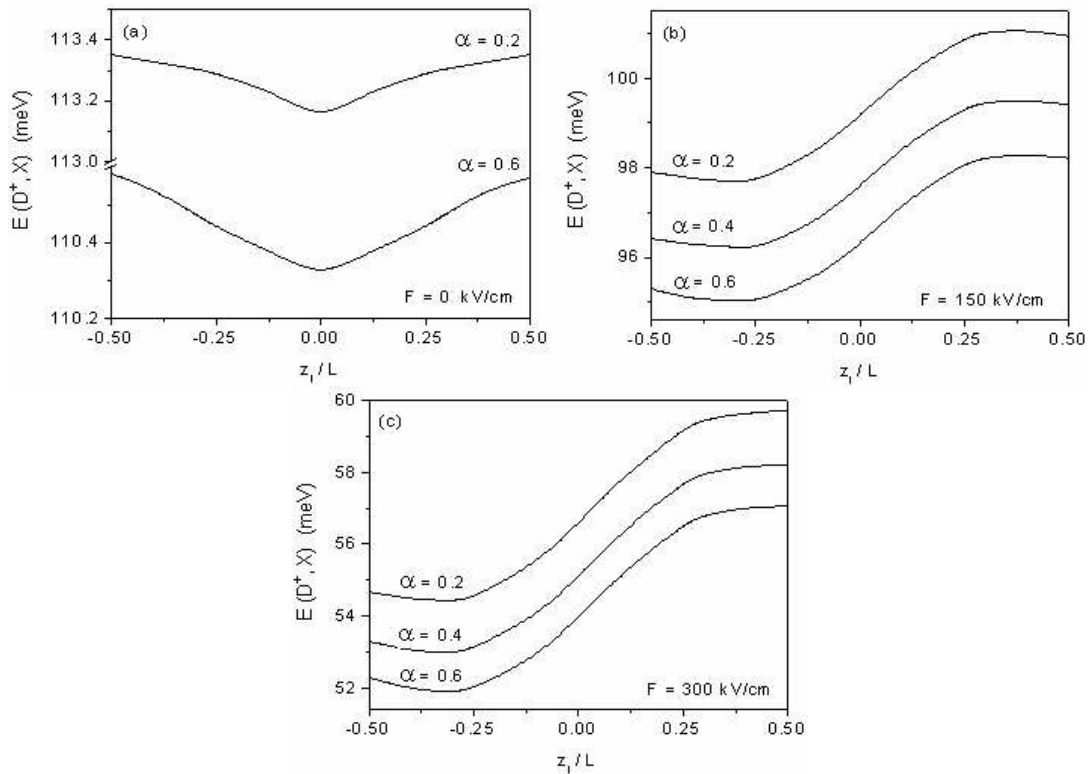
Fig. 1. The energy $E(D^+, X)$ of the exciton complex in a $L=10$ nm GaAs-AlGaAs PQW for (a) F = 0 kV/cm, (b) F = 150 kV/cm and (c) F = 300 kV/cm, as a function of the impurity position and with different values of the effective screening parameter α.

The energy $E(D^+, X)$ of the exciton complex as a function of the impurity position along the z axis, with and without electric field, and for different values of the effective screening parameter, is shown in Fig. 1. From our calculation, we found a ratio of around 4% for the first-order energy correction relative to the unperturbed energy for the ground state. The second-order energy corrections are not expected to be significant, especially for weaker electric fields, i.e., in the case of a strong quantum confinement.

It is observed that for zero electric field (Fig. 1(a)), the exciton states corresponding to symmetrical position of the impurity are degenerated and their energy takes larger values as the impurity moves away from the well center. Since the wave function for the 1S state decays away from the well center, when the donor moves towards the well edge the average donor ion-electron separation increases and the dominant perturbing term V_c^e decreases. Fig. 1(a) shows a weak

dependence of the energy with z_i for this narrow PQW, because the quantum confinement effect overrides the effect of the donor position change.

For $F \neq 0$ (Figs. 1(b) and 1(c)), unlike the monotonic behavior observed in the absence of the field, the curves of exciton complex energy reveal a peak for donors at the right side of the QW. This is due to the fact that in electric field the hole is pushed in the right side of the well, so that for $z_i > 0$ the main contribution to the perturbing term comes from the screened potential V_c^h. This positive quantity first increases with z_i (until the donor position coincides with the maximum of the hole probability density z_{0h}, and the curve of $E(D^+, X)$ shows a peak), and then decreases. For the $L = 10$ nm GaAs-AlGaAs PQW we found a $z_{0h} \cong 4$ (5) nm when $F = 150$ (300) kV/cm. Conversely, for $z_i < 0$, the attractive term V_c^e in Eq. (7) dominates the weakening of the $E(D^+, X)$. The curves of Figs. 1(b) and 1(c) show a minimum around $z_{0e} \cong -2.5$ (- 3.0) nm for $F = 150$ (300) kV/cm, when the electron probability density is at the maximum and the complex exciton energy is at the minimum.

We note that the variation of $E(D^+, X)$ with z_i becomes significant for higher values of the electric field, when the hole wave function has a large penetration into the barriers (Fig.1(c)). As expected, the maximum of the probability density for hole (determined by the competition between the barrier potential, the Coulomb interaction electron-hole and the electric field effect) changes more significantly with F than that of the electron.
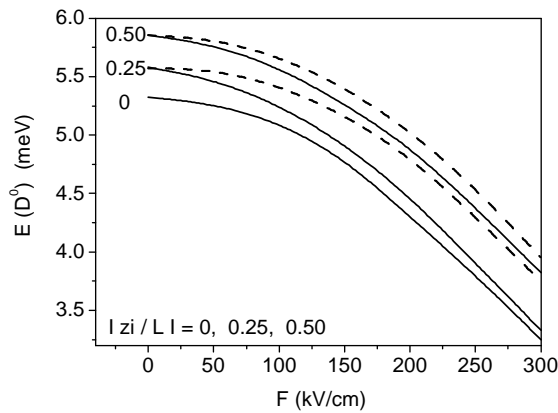

Fig. 2. The neutral donor ground-state energy as a function of the applied electric field for $|z_i|/L = 0, 0.25$, and 0.50. $z_i < 0$: solid lines; $z_i > 0$: dashed lines.

The neutral donor ground state energy $E(D^0)$ as function of the applied electric field, for different impurity positions along z-axis is shown in Fig. 2. It is observed that the ground state energy decreases as the applied electric field is increased. For sufficient large F the degeneracy of the donor states symmetrically positioned is broken because the electron probability density along the z-axis varies in the presence of an applied field. As expected, in the applied electric field, the ground state energy of the donor impurity is highest (lowest) when the impurity is located in the right (left) side of the well, due to the increasing (decreasing) of the separation between the donor and the electron.

Fig. 3 shows the behavior of the binding energy E_b for the exciton complex as a function of the electric field in a GaAs-AlGaAs PQW for effective screening parameter $\alpha = 0.2$ and $\alpha = 0.6$, respectively, and for different impurity positions. In the presence of the electric field, the electron and the hole are spatially separated along the z direction. As they are pushed in the opposite directions, their Coulomb attraction and consequently, the binding energy decreases. From the same figure, it is observed that the decrease of the binding energy is larger for an impurity position at the right side of the QW (see also Fig. 4). Accordingly to the stability conditions [9], positive binding

energy means essentially that the mean value of the attractive interaction between electron and hole is greater than the mean value of the repulsive potential between hole and donor impurity. For $z_i > 0$, as F increases, the repulsive potential between hole and donor impurity is enhanced, the hole is more free to move away from the complex and thus the system is more unstable.
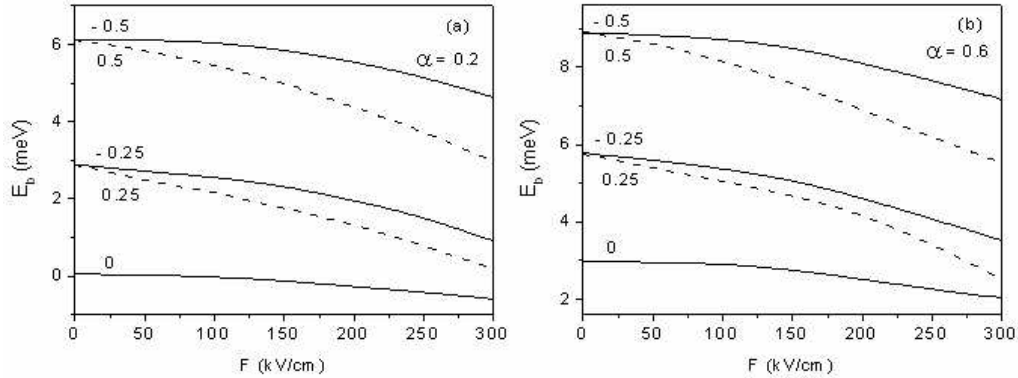

Fig. 3. The electric field dependence of the binding energy of the exciton complex in a GaAs-AlGaAs PQW with $L = 10$ nm for different impurity positions and (a) $\alpha = 0.2$; (b) $\alpha = 0.6$. $z_i / L < 0$: solid lines; $z_i / L > 0$: dashed lines.

For small electric fields (F $\leq$ 70 kV/cm) for all values of z_i, it appears that $E_b > 0$, so that we get a stable binding. This result is consistent with theoretical values obtained by Essaoudi *et al.* [9] for GaAs-$Al_{0.30}Ga_{0.70}As$ *square quantum well* with $L = 10$nm. However, for higher values of the field (F $\geq$ 100 kV/cm) and the effective screening parameter $\alpha \leq 0.3$, the complex becomes unstable when the impurity is located near the well center (see also Fig. 5(a)).
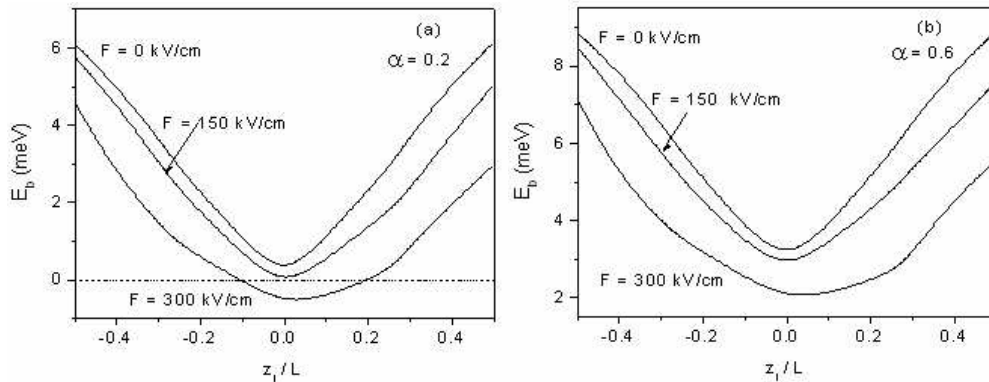

Fig. 4. Variation of the exciton complex binding energy as a function of the impurity position for three values of the applied electric field.

The curves of E_b versus z_i in Fig. 4 show a minimum for $z_i = 0$ and a monotonical increase with donor position away from the center of the well. From our calculation, we found that for $F = 0$, this dependence comes from the $E(D^0)$ behavior, the contribution from the perturbing term being small compared to the neutral donor energy. When an electric field is applied, $E^{(1)}$ (and hence $E(D^+, X)$) is substantially decreased for $z_i < 0$, and slightly increases when the donor is located at the right side of the QW. Because the $E(D^0)$ energy is less sensitively to F (see Fig. 2), the symmetry in the binding energy is broken; E_b takes larger values for $z_i < 0$, when the system is

more stable. The difference $\Delta E_b = E_b(-z_i) - E_b(z_i)$ increases with F and α and is quite large for the distances z_{0i} $(i = e, h)$ implying greater confinement of the electron (hole) around the impurity position. Accordingly with our above discussion we observe that for sufficiently large electric fields, in all studied cases, for on-center donor position we obtain unbound states for the exciton complex. E_b increases when $|z_i|$ increases until the bound state appears for impurity position greater than a critical value z_c. This critical distance strongly depends on the screening parameter and, as we can see from Fig. 4, z_c increases with F. The z_i dependence of the binding energy shows that a single Coulomb center with a proper position can largely change the exciton spectrum of a quantum well and, then, the electronic and optical properties. The concept might be useful for designing some devices in the future.
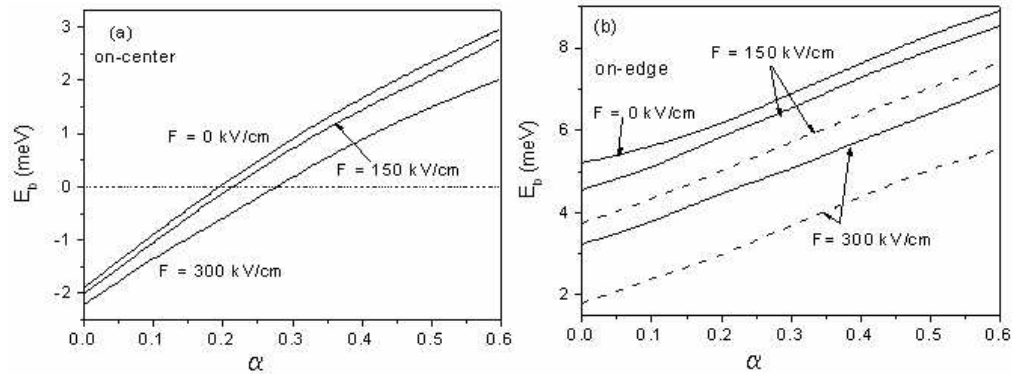

Fig. 5. The binding energy of the (D^+, X) complex as a function of the effective screening parameter α for on-center (a) and on-edge (b) donors. $z_i < 0$: solid lines; $z_i > 0$: dashed lines.

The effect of the screening parameter α on the binding energy E_b for three electric fields is represented in Fig. 5 for on-center and on-edge donors in a GaAs–AlGaAs PQW with $L = 10$ nm. It is clear that in both cases the binding energy of the exciton complex increases, as expected, with a reduced Coulomb repulsion resulting from the larger values of α. However, there is a difference in the magnitude of the effect between the two-donor positions. An increase of the screening parameter in vicinity of the donor implies a localized decrease in the repulsive interaction between the hole and the donor. For $F = 0$, when the donor is localized in the center of the well, this position coincides with the peak in the probability distribution of the hole. Consequently, the change of the parameter α leads to a large variation of the exciton complex binding energy. Conversely, when the donor is located at the right (left) edge of the well ($z_i / L = \pm 0.5$), the localized decrease in the Coulomb repulsion occurs in a region which is spatially separated from the peak in the hole probability distribution and hence the effect of the screening parameter is correspondingly reduced. When an electric field is applied, the position of the peak in the hole probability distribution is shifted toward the right edge of the well. Consequently, in the strong electric fields, the spread of the binding energy for the center donor is smaller than that of the edge donor.

4. Conclusions

By means of the effective-mass approximation and within a perturbation- variational procedure we have calculated the binding energy of the ground state of an exciton bound to an ionized donor in a GaAs-AlGaAs PQW with a longitudinal electric field. The dependence of the exciton complex energy as a function of the applied electric field, the donor-impurity position, and the screening parameter for the donor-hole interaction has been analyzed. We found that the electric field breaks down the degeneracy of symmetrically positioned impurities. Our results show that the

applied electric field is determinant for the existence of bound states for the exciton complex, together with the impurity position and the screening parameter value. These aspects must be taken into account in the interpretation of optical phenomena related to excitons bound to the ionized donor in the PQWs, in which the effect of the applied electric field competes with the strong quantum confinement.

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