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Quantum-confined Stark effects of an exciton bound to an ionized donor in a GaAs/Ga$_{1-x}$Al$_x$As quantum well

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We have calculated by a variational procedure the binding energy of an exciton bound to an ionized donor (D^+,X) in a GaAs/Ga$_{1-x}$Al$_x$As quantum well with $x=0.15$ and $x=0.30$ as a function of the well width L and an electric field F perpendicular to the well interfaces. The dependence of the correlation energy on the electric field is investigated and compared with those of a shallow donor D^0 and an exciton X. It is shown that the correlation energy of the (D^+,X) complex decreases monotonically at increasing F values in the case of large well widths ($L \gtrsim 10$ nm). However, it is not sensitive to the electric field in narrow QW's. For all investigated well widths, the (D^+,X) complex remains stable compared to its product of dissociation.

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I. INTRODUCTION

The electric field effects on insulating quantum well structures have received, in the last years, much interest due to the possibility of making fast electro-optic devices. It has been shown that the electronic properties of quantum well (QW) systems may change significantly when an electric field is applied along the growth direction.[1] Both the induced polarization and the energy level shift of the confined carriers are responsible for the intensity decrease and peak shift of the photoluminescence (PL) spectra observed in GaAs/Ga$_{1-x}$Al$_x$As multi-quantum-well structures.

Theoretically, the electric field F effects on the energy of confined electrons and holes were studied by variational and exact numerical calculation by Bastard *et al.*[2] and Austin *et al.*[3] Later, Brum and Bastard[4] extended the calculations to Wannier excitons states and showed that their binding energies are little affected by F in narrow QW's. However a significant reduction of the exciton binding energy occurs in QW structures with larger well widths L ($L \gtrsim 100$ Å)). Brum and Priester[5] reported the electric field dependence on the binding energy of shallow donors in GaAs/Ga$_{1-x}$Al$_x$As QW's for different well widths and impurity positions. Recently Dujardin *et al.*[12] studied the influence on an electric field on the energies of a negatively charged excitons in semiconductor quantum wells. They found that the correlation energy, defined as the difference between the energy associated with the relative motion and that of the three free particles, increases with the electric field strength and with the well width. However, for narrow wells, the correlation energy is little affected as it has shown in the case of excitons. To our knowledge, there does not exist any work concerning the influence of an electric field on an exciton-ionized-donor (D^+,X) complex in a semiconductor quantum well.

Historically its possible existence in three-dimensional (3D) semiconductors was predicted in 1958 by Lampert.[6] In 3D semiconductors its stability and binding energies have been the subject of several theoretical studies.[7,8] As a result, it appears[9] that the (D^+,X) complex is stable if the effective mass ratio $\sigma=m_e^*/m_h^*$ satisfies the condition $\sigma\leqslant\sigma_c^{3\mathrm{D}}=0.426$. However, in the two-dimensional (2D) case, Stauffer and Stébé[10] have shown that the (D^+,X) complex remains stable until $\sigma\leqslant\sigma_c^{2\mathrm{D}}=0.88$, a value about two times larger than that obtained in the 3D case. Erzhen *et al.*[11] calculated the binding energy of a (D^+,X) complex with a donor located on the surface of a nonpolar semiconductor in function of σ and the high-frequency dielectric constant ϵ_∞ of the host semiconductor occupying the semi-infinite space. They showed that the binding energy of the complex decreases with both σ and ϵ_∞ and that no unstable range of σ appears. Stébé *et al.*[13,14] extended their 3D and 2D calculations to the case of an exciton bound to an ionized impurity located at the center of a GaAs/Ga$_{1-x}$Al$_x$As single QW with $x=0.15$ and $x=0.30$. They concluded that the binding energy lies in the range between the 3D and 2D cases.

In the present work, we study the influence of an applied electric field on the binding energy of an exciton bound to an ionized donor in GaAs/Ga$_{1-x}$Al$_x$As QW's. We use the effective mass approximation and adopt a trial envelope wave function extending that used previously[13,14] without any external field. In the next section we outline our method of calculations. Our results are reported in Sec. III.

II. THEORY

We consider a (D^+,X) complex located at the center of a GaAs/Ga$_{1-x}$Al$_x$As single quantum well in the presence of a uniform electric field F perpendicular to the well interface. In the envelope function approximation the Hamiltonian reads

$$H_{(D^+,X)}=\epsilon_g-\frac{1}{2}\Delta_e-\frac{\sigma}{2}\Delta_h-\frac{1}{r_e}+\frac{1}{r_h}-\frac{1}{r_{eh}}+V_w^e+V_w^h+f(z_e-z_h), \tag{1}$$

$$V_w=\sum_{i=e,h}V_i\,\theta\left(z_i^2-\frac{L^2}{4}\right). \tag{2}$$

Here V_w^i $(i=e,h)$ are the electron and hole quantum well potentials with the well width L. V_e and V_h are the electron and hole band offsets. $\theta(x)$ is the Heavyside unit-step function and ϵ_g corresponds to the energy gap the well material. r_e, r_h, and r_{eh} are the (electron, hole)-ionized donor distances, and electron-hole distance. We used effective atomic units with a length unit equal to the 3D donor effective Bohr radius, $a_D=\kappa\hbar^2/e^2m_e^*$, and an energy unit equal to twice the absolute value of the 3D donor Rydberg, $2R_D=\hbar^2/m_e^* a_D^2$. $f=F/F_0$ is a dimensionless parameter for the electric field intensity, where $F_0=e/\kappa a_D^2$ is the unit of the electric field. We neglect band nonparabolicity and both differences of the effective masses and dielectric constants between the well and barrier materials.

We determine the ground state energy using the variational method. In the case of an electric field parallel to the growth direction, the symmetry of the problem is not modified comparatively to the case with no external field. Thus we use a trial wave function analogous to that we used previously[13] in the study of the (D^+,X) complex in a semiconductor QW. However, in the present case, we replace the electron and hole QW ground states wave functions by the corresponding functions taking to account the existence of an external electric field analogous to that obtained by Brum and Bastard.[4] Thus our trial wave function reads

$$\psi(r)=\mathcal{N}_{(D^+,X)}\chi_e(z_e)\chi_h(z_h)\sum_{lmnpr} C_{lmnpr}a_p(z_e)b_r(z_h) \times\exp\left(-\frac{ks}{2}\right)s^l u^m t^n, \tag{3}$$

$$a_p(z_e)=z_e^p\exp(-\alpha_e z_e^2) \quad \text{and} \quad b_r(z_r)=z_h^r\exp(-\alpha_h z_h^2), \tag{4}$$

$$\chi_e(z_e)=\begin{cases} A_e\exp(-\beta_e z_e)\exp(-q_e|z_e|) & \text{if} \quad |z_e|>L/2,\\ B_e\exp(-\beta_e z_e)\cos(k_e z_h) & \text{if} \quad |z_e|\leqslant L/2,\end{cases} \tag{5}$$

$$\chi_h(z_h)=\begin{cases} A_h\exp(\beta_h z_h)\exp(-q_h|z_h|) & \text{if} \quad |z_h|>L/2,\\ B_h\exp(\beta_h z_h)\cos(k_h z_h) & \text{if} \quad |z_h|\leqslant L/2.\end{cases} \tag{6}$$

$\mathcal{N}_{(D^+,X)}$ stands for the normalization constant. $\chi_i(z_i)$ $(i=e,h)$ are the ground state wave functions of an electron or a hole in a QW subjected to an electric field parallel to the growth axis. The constants A_i and B_i $(i=e,h)$ are determined by the continuity conditions for the $\chi_i(z_i)$ functions and their derivatives at $z_i=\pm L/2$. The vectors k_e, q_e (k_h, q_h) are the characteristic wave vectors for the ground-state QW electron (hole) wave functions at zero electric field $k_e=\sqrt{2E_e}$, $k_h=\sqrt{(2/\sigma)E_h}$, $q_e=\sqrt{2(V_e-E_e)}$, $q_h=\sqrt{2/\sigma(V_h-E_h)}$. E_e and E_h are the confinement energies of the lowest electron and hole QW bound states. β_e and β_h are variational parameters which depend on the electric field strength and are determined in the case of simple electron and hole problem.

The in-plane part of our wave function depends on the Hylleraas type coordinates s, t and u defined by

$$s=\rho_e-\rho_{eh}, \quad t=\rho_e+\rho_{eh}, \quad u=\rho_h,$$
$$0\leqslant s, \quad -u\leqslant t\leqslant u, \quad 0\leqslant u\leqslant s, \tag{7}$$

where ρ_e, ρ_h, and ρ_{eh} are the electron and the hole coordinates in the plane perpendicular to the growth axis. l, m, n, p, and r are positive integers or zero.

The linear variational parameters C_{lmnqr} as well as the three nonlinear parameters α_e, α_h, and k are determined by minimizing the mean value of the total energy

$$E=\min_{\alpha_e,\alpha_h,k}\frac{\langle\psi|H_{(D^+,X)}|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{8}$$

So they must satisfy the conditions $\partial\langle H_{(D^+,X)}\rangle/\partial k=\partial\langle H_{(D^+,X)}\rangle/\partial\alpha_e=\partial\langle H_{(D^+,X)}\rangle/\partial\alpha_h=\partial\langle H_{(D^+,X)}\rangle/\partial C_{lmnpr}=0$, for all possible values of the indices l,m,n,p,r. The last equation is equivalent to the eigenvalue problem

$$(\mathbf{H}-E\mathbf{S})\mathbf{C}=0, \tag{9}$$

where $\mathbf{C}$ denotes the column matrix of the linear coefficients C_{lmnpr}. The matrix $\mathbf{H}$ and $\mathbf{S}$ are defined with respect to the basic functions defined above.

III. NUMERICAL RESULTS AND DISCUSSION

In order to study the stability of the (D^+,X) complex against dissociation into the most stable dissociation products

$$(D^+,X)\rightarrow D^0+h,$$
$$(D^+,X)\rightarrow X+D^+, \tag{10}$$

it is necessary to know the values of the ground state of the neutral donor D^0 and the exciton X with the same accuracy as the exciton-ionized donor energy E. To this purpose we have performed a variational calculations for both neutral donor and exciton using the following trial waves functions:

$$\psi_{D^0}=\mathcal{N}_{D^0}\chi_e(z_e)\sum_p C_p z_e^p\exp(-\alpha_e z_e^2)\exp(-k\rho), \tag{11}$$

$$\psi_X=\mathcal{N}_X\chi_e(z_e)\chi_h(z_h)\sum_{pr} C_{pr}z_e^p\exp(-\alpha_e z_e^2)z_h^r \times\exp(-\alpha_h z_h^2)\exp(-k\rho), \tag{12}$$

where ρ is the in-plane separation of the electron-hole pair in the case of the exciton and the in-plane electron-ionized donor distance in the case of the donor. α_e, α_h, and k as well as C_p and C_{pr} are variational parameters. p and r are positive integers or zero. After some preliminary computations, we have obtained the required accuracy with a three terms wave function for the neutral donor, i.e., $p\leqslant 2$, and a six-terms wave function for the exciton, i.e., $p+r\leqslant 2$.

It is useful to define the "correlation energies" by

$$E_c^{(D^+,X)}=E_{(D^+,X)}-\mathcal{E}_e-\mathcal{E}_h\,, \qquad (13)$$

$$E_c^X=E_X-\mathcal{E}_e-\mathcal{E}_h\,, \qquad (14)$$

$$E_c^{D^0}=E_{D^0}-\mathcal{E}_e\,, \qquad (15)$$

where E_{D^0} and E_X correspond, respectively, to the ground state energies of the neutral donor and of the exciton. $\mathcal{E}_e$ and $\mathcal{E}_h$ are the energies of the electron and the hole in a QW in the presence of an electric field F. Thus the stability conditions of the (D^+,X) complex may be written

$$E_{(D^+,X)}\leqslant E_{D^0}\Leftrightarrow E^c_{(D^+,X)}\leqslant E^c_{D^0}\,, \qquad (16)$$

$$E_{(D^+,X)}\leqslant E_X\Leftrightarrow E^c_{(D^+,X)}\leqslant E^c_X\,. \qquad (17)$$

We compute the binding energy of the (D^+,X) complex as a function of the well width L, the mass ratio σ, the electric field intensity F, and the conduction and valence bands offsets V_e and V_h. In the presence of the electric field, odd and even terms are necessary to express the polarization. However, at zero field, due to the existence of the inversion symmetry along the growth axis, the wave function must have definite parity, and for the ground state only the even order terms have to be taken into account. We have first determined the nonlinear variational parameters k, α_e, and α_h using a ten-term wave function defined by the conditions $l+m+n\leqslant 2$ and $p+r=0$. In the present study, keeping fixed these predetermined values of k,α_e, and α_h, we use a 112-term wave function defined by the conditions $l+m+n\leqslant 5$ and $(pr)=00,11$. This choice corresponds to a realistic compromise between accuracy and computing time.

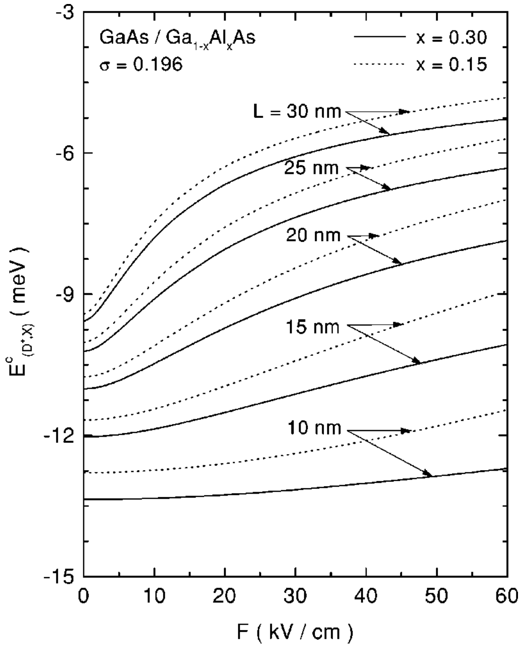

FIG. 1. Electric field dependence of the(D^+,X) complex correlation energies in a GaAs/Ga$_{1-x}$Al$_x$As QW ($x=0.15$ and 0.30) for different values of the well thickness ($L=10$, 15, 20, 25, and 20 nm).

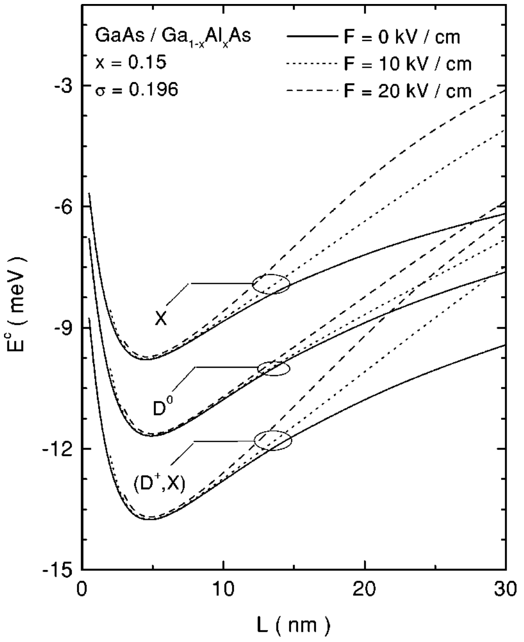

FIG. 2. Calculated dependence of the correlation energies of the shallow donor impurity, the exciton and the (D^+,X) complex in a GaAs/Ga$_{1-x}$Al$_x$As QW with $x=0.15$, versus the GaAs well thickness L, for three values of the electric field F=0, 10, and 20 kV/cm).

We have done our numerical calculations in the case of a GaAs/Ga$_{1-x}$Al$_x$As QW. We use the following material data:[15,16] $m_e^*/m_0=0.0665$, $m_{hh}^*/m_0=0.34$, and $\kappa=12.5$. The heavy hole mass has been proposed[15] in order to fit experimental observations in both parabolic and square GaAs QW's. We remark that this value lies between the theoretical in-plane and the perpendicular values 0.11 and 0.38, obtained using the Luttinger parameters $\gamma_1=6.85$, $\gamma_2=2.10$, and $\gamma_3=2.90$. Nevertheless, it must be stressed that in the present work we have not taken into account the possible difference between the barrier and well materials. The bands offsets are given by $V_e=Q_e\Delta\epsilon_g$ and $V_h=Q_h\Delta\epsilon_g$, where $Q_e=0.57=1-Q_h$. Furthermore, we assume that the band gap difference $\Delta\epsilon_g$ and the Al concentration x are related by[17] $\Delta\epsilon_g=1.155x+0.37x^2$ eV. In this case we get $\sigma=0.196$ for the effective mass ratio, $a_D=9.95$ nm for the effective neutral donor Bohr radius and 2 Ry$=11.58$ meV for twice the effective neutral donor Rydberg, and $F_0=11.638$ kV/cm for the electric field unit.

In Fig. 1 we show the electric field dependence of the correlation energy of (D^+,X) for different values of the well width ($L=10$, 15, 20, 25, and 30 nm) with aluminum concentrations $x=0.15$ and $x=0.30$. We note that the correlation energy increases with the field intensity. This increase is negligible for narrow wells ($L\simeq 10$ nm) because the quantum confinement effect overrides that of the electric field, but become significant for higher values of the width ($L\gtrsim 20$ nm).

Figure 2 shows the calculated correlation energies of the (D^+,X) complex, the exciton and the shallow donor impurity, as functions of the well width, for three values of the

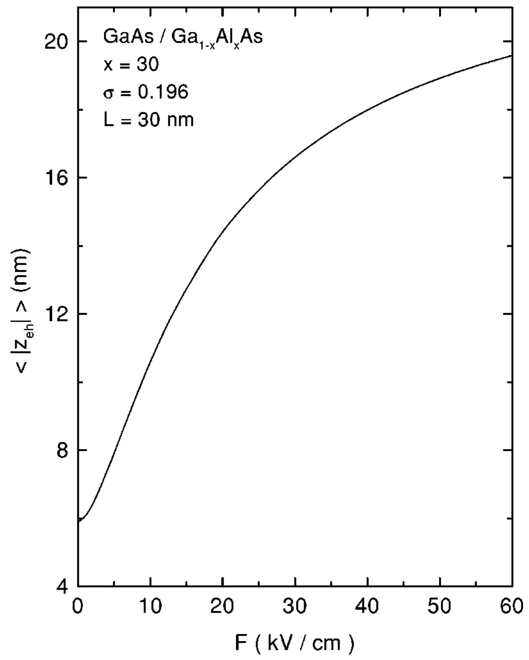

FIG. 3. Variation of the electron-hole pair average z separation $\langle|z_{eh}|\rangle$ in the (D^+,X) complex as a function of the electric field intensity for $x=0.30$ and $L=30$ nm.

electric field intensity $F=0$, 10, and 20 kV/cm). At zero electric field, when L decreases, the correlation energies of the three systems first decrease because of the confinement effects, and subsequently they increase because the spread out of the wave functions outside the well. We remark that the correlation energies of the three systems are not sensitive to the strength of the electric field in the vicinity of the minimum ($L\simeq5$ nm). When the width of the well increases, the correlation energies remain negative for the three values of the field intensity. For all values of the field intensity in the range [0,20 kV/cm] and for $L\leqslant30$ nm, it appears that $E^c_{(D^+,X)}/E^c_{D^0}>1$ and $E^c_{(D^+,X)}/E^c_X>1$. Thus in these cases the complex is stable against dissociation.

In Fig. 3 we show the variation of the electron-hole pair average z separation $\langle|z_{eh}|\rangle$ in the (D^+,X) complex as a function of the electric field intensity for $x=0.30$ and $L=30$ nm. It appears that, as expected, this separation increases with the electric field. Indeed, the electric field tends to repel the electron and the hole towards the opposed interfaces. This leads to a reduction of the Coulombic potential energy and of the absolute value of the correlation energy.

In order to estimate the position of the (D^+,X) lines, it is necessary to make a hypothesis concerning the radiative process involved in the transition. The most simple one consists in a transition between an initial state involving an ionized impurity D^+ and a (D^+,X) final state. The energy balance corresponding to direct transitions reads

$$h\nu_{(D^+,X)}=h\nu_X+E^c_X-E^c_{(D^+,X)}, \tag{18}$$

where $h\nu_{(D^+,X)}$ and $h\nu_X$ are, respectively, the ionized donor bound exciton and exciton transition energies. In order to give an estimation of the localization energy $\Delta h\nu=h\nu_X-h\nu_{(D^+,X)}$, we compare in Fig. 4 the exciton and bound exciton correlations energies for different values of the well width as functions of x and for $F=20$ kV/cm. We remark that the localization energy is little affected by the aluminum concentration x because the quantum confinement for the exciton and for the (D^+,X) complex are of the same order. On the other hand, when L increases, $\Delta h\nu$ decreases.

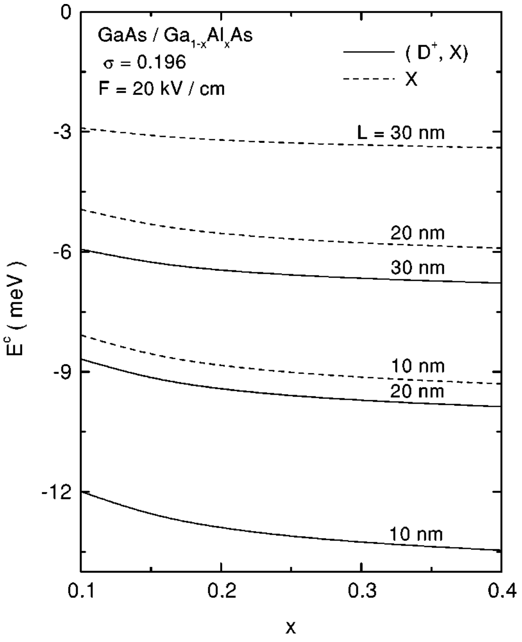

FIG. 4. Variations of the correlation energies of the exciton X and the (D^+,X) complex in the case of a GaAs/Ga$_{1-x}$Al$_x$As QW as functions of the Al concentration x for $F=20$ kV/cm and for different values of well width L.

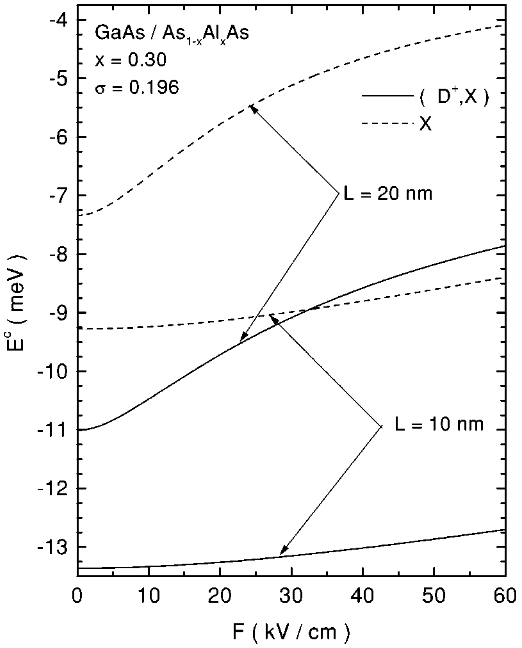

FIG. 5. Electric field dependence of the exciton and the correlation energies of the exciton and the (D^+,X) complex on the correlation energies in a GaAs/Ga$_{1-x}$Al$_x$As QW with $x=0.30$ for two values of the well thickness ($L=10$ and 20 nm).

In order to show the effect of the electric field on the localization energy $\Delta h\nu$, we show in Fig. 5 the variations of the correlation energies of the (D^+,X) complex and the exciton as functions of the electric field intensity for two values of the well width ($L=10$ and 20 nm). As a result, $\Delta h\nu$ is not sensitive to electric field. The two last figures may be used to determine the location of the (D^+,X) line relative to the exciton line.

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