Density of states and optical-absorption spectra of shallow impurities in quantum wells under the influence of a longitudinal electric field

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We have calculated the densities of states and the optical-absorption spectra of shallow donors and acceptors in GaAs-(Ga,Al)As quantum wells under the influence of a constant electric field applied parallel to the growth axis. The impurity binding energies were calculated as functions of the impurity position in a quantum well of infinite depth, where we have used a variational procedure within the effective-mass approximation. The main feature found was a quenching of one of the peaks due to interface impurities at moderate electric fields. We compare these optical-absorption spectra with previous calculations in the absence of an electric field.

I. INTRODUCTION

Since Bastard[1] calculated for the very first time the hydrogenic impurity states in quantum wells (QW's) many works on this subject have been published. Mailhot, Chang, and Damen[2] and Greene and Bajaj[3] have performed some improvements by calculating the ground state and the first excited states for QW's of finite depth. Variational calculations for $n=1$ levels with electric fields were performed by Bastard *et al.*[4] and for the binding energies of shallow impurities by Brum, Priester, and Allan.[5] Oliveira and Falicov[6] have calculated the density of impurity states and gave a correct interpretation of these results. Recently, Oliveira and Pérez-Alvarez[7,8] have studied the impurity-related optical-absorption properties for QW's.

Chemla *et al.*[9] measured electroabsorption spectra for weak electric fields (about 16 kV/cm) for multiple quantum wells, whereas Wood *et al.*[10] performed similar measurements studying high-speed optical modulation with QW's.

In this work we calculate the effect of a longitudinal electric field on the densities of impurity states and on the optical-absorption spectra due to hydrogenic impurities in QW's. The impurity binding energies are calculated within a variational scheme in the effective-mass approximation. From the binding energies we obtain the densities of impurity states and the transition probability per unit time between the $n=1$ valence (conduction) subband and the donor (acceptor) impurity band. In this work we are concerned only with GaAs-(Ga,Al)As QW's of infinite depth.

In Sec. II we discuss the theoretical aspects of this work, results and discussion are presented in Sec. III, and conclusions in Sec. IV.

II. THEORY

We consider a QW of infinite depth and use a Hamiltonian in the effective-mass approximation for the shallow impurity

$$H=H_0+H_I\ , \tag{2.1}$$

where H_0 is

$$H_0=-\frac{\hbar^2}{2m^*}\frac{\partial^2}{\partial z^2}+V(z)+|e|Fz\ , \tag{2.2}$$

where F is the applied longitudinal electric field,

$$V(z)=\begin{cases}0, & |z|<L/2\\ \infty, & |z|>L/2\ ,\end{cases} \tag{2.3}$$

and

$$H_I=-\frac{\hbar^2}{2m^*}\nabla_\perp^2+\frac{e^2}{\epsilon_0[x^2+y^2+(z-z_i)^2]^{1/2}}\ , \tag{2.4}$$

with z_i being the impurity position along the growth axis and ϵ_0 the dielectric constant.

The ground-state wave function $\phi_0(z)$ is chosen as[4]

$$\phi_0(z)=N_0(\beta)\cos\left[\frac{\pi z}{L}\right]\exp\left[-\frac{\beta z}{L}\right]\ . \tag{2.5}$$

The above wave function describes the situation in which the particle is pushed against an interface and, at high fields, the charge distribution is concentrated near the well barrier. The variational parameter β in Eq. (2.5) will introduce the effect of the electric field through the exponential function and $N_0(\beta)$ is a normalization constant. The $n=1$ energy level $E_0(\beta)$ for a given field strength F is then[4]

$$E_0(\beta)=\frac{\pi^2}{L}\left[1+\frac{\beta^2}{\pi^2}\right]+|e|Fz\left[\frac{1}{2\beta}+\frac{\beta}{\beta^2+\pi^2}-\frac{1}{2}\coth\beta\right]\ , \tag{2.6}$$

where we have already introduced effective reduced units

so that $\hbar=1$, $\epsilon_0=1$, and $m^*=\frac{1}{2}$ and results are then given in units of effective rydbergs $\mathcal{R}_0^*=5.72$ meV (26 meV) and effective Bohr radius $a_0^*\simeq 100$ Å (22 Å) for electrons (holes) with a dielectric constant $\epsilon_0=12.58$.

The trial impurity wave function is chosen as a $1s$-like wave function

$$\psi(\mathbf{r})=N\phi_0(z)\exp[-(x^2+y^2)^{1/2}\lambda] . \tag{2.7}$$

The resulting binding energy is then

$$E_i(\lambda)=E_0(\beta)+\frac{1}{\lambda^2}-\frac{8}{\lambda^2}\int_{-L/2}^{+L/2}|\phi_0(z)|^2\left\{\frac{\pi}{2}\left[\mathcal{H}_1\left[\frac{2|z-z_i|}{\lambda}\right]-N_1\left[\frac{2|z-z_i|}{\lambda}\right]\right]-1\right\}|z-z_i|\,dz , \tag{2.8}$$

where $\mathcal{H}_1$ and N_1 are the first Struve and Neumann functions.

If the QW is not too thin, one may treat the impurity position z_i as a continuous random variable, and provided that there is no intentional doping, define a density of impurity states per unit binding energy[1] $g_L(E_i)$ as

$$g_L(E_i)=\frac{1}{L}\sum_{\{z_i\}}\left|\frac{\partial E_i}{\partial z_i}\right|^{-1} , \tag{2.9}$$

where $\{z_i\}$ are all impurity positions with the same impurity binding energy E_i. In the absence of an electric field ($F=0$) the summation can be replaced by a factor of 2.

The transition probability per unit time for valence to donor transitions (associated to a single impurity located at $z=z_i$) is proportional to the square of the matrix element of the electron-photon interaction H_{int} between the wave function of the initial (valence) and final (donor) states, i.e.,

$$\tau^{-1}=\frac{2\pi}{\hbar}\sum_i|\langle f|H_{\text{int}}|i\rangle|^2\delta(E_{\text{final}}-E_{\text{initial}}-\hbar\omega) , \tag{2.10}$$

following a similar "golden-rule" approach as used by Bastard[1] and later by Oliveira and Pérez-Alvarez.[7,8]

The final result of the transition probability as function of the length of the QW, the position z_i of the impurity and the energy of the photon $\hbar\omega$ is

$$\tau_L^{-1}(z_i,\omega)=\tau_0^{-1}\left[\frac{a_0^*}{a_0}\right]\left[\frac{m_v}{m_0}\right]\left[\frac{a_0^3}{L}\frac{|J|^2}{\lambda^2 a_0^3}\right]_{k_\perp}Y(\Delta) , \tag{2.11}$$

where a_0 is the Bohr radius, a_0^* is the effective Bohr radius [$a_0^*=\hbar^2\epsilon_0/(m^*e^2)$] and $Y(\Delta)$ is the unit step function.

We have also the following definitions:

$$\Delta=\hbar\omega-\mathcal{E}_g+E_i(\lambda) , \tag{2.12}$$

$$k_\perp=(2m_v\Delta/\hbar^2)^{1/2} , \tag{2.13}$$

$$\mathcal{E}_g=E_g+E_{n=1}^c(F)+E_{n=1}^v(F) , \tag{2.14}$$

$$\tau_0^{-1}=\frac{2m_0}{\hbar^3}a_0^2|\mathbf{c}|^2|\mathbf{c}\cdot\mathbf{k}|^2 , \tag{2.15}$$

where E_g is the bulk GaAs band gap and $E_{n=1}^c$ ($E_{n=1}^v$) is

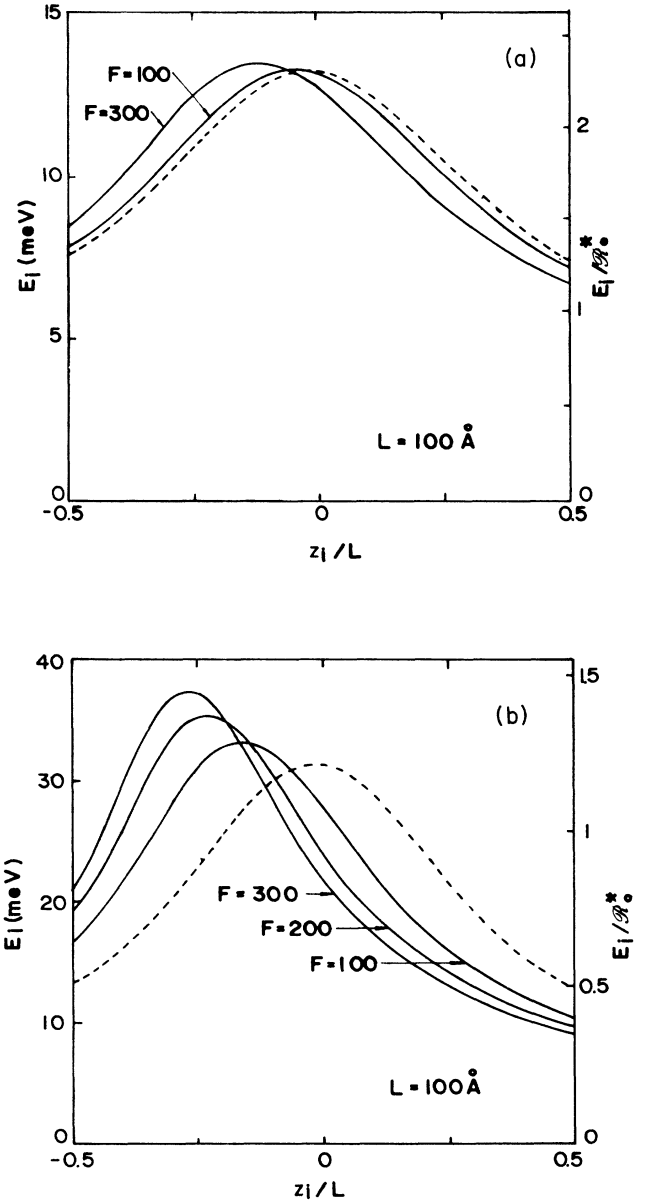

FIG. 1. Binding energies of (a) donors and (b) acceptors as functions of the impurity position z_i, in a QW with $L=100$ Å, for several values of the electric-field intensity F (in kV/cm) and in the absence of an electric field (dashed lines). The fields in (a) and (b) are in opposite directions.

the bottom (top) of the first conduction (valence) subband. The constant τ_0^{-1} is taken in the same manner as in the work of Oliveira and Pérez-Alvarez[7,8] so that we could compare their results and ours directly.

For an infinite QW with wave functions given by (2.5) and (2.7) we obtain

$$J=\frac{2\pi}{\alpha^3\lambda}\frac{N_0(\beta)}{N_0^2(\beta/2)}\ , \tag{2.16}$$

where

$$\alpha=(k_\perp^2+1/\lambda^2)^{1/2}\ . \tag{2.17}$$

Using the same suppositions as we have used for the density of impurity states, the total transition probability per unit time is then given by

$$\tau^{-1}(\omega)=\frac{1}{L}\int_{-L/2}^{+L/2}\tau_L^{-1}(z_i,\omega)\,dz_i\ . \tag{2.18}$$

The transition probability for transitions from the acceptor subband to the first conducting subband is obtained in an analogous way as in Eq. (2.11), changing only m_v to m_c.

III. RESULTS AND DISCUSSION

In Fig. 1(a) we display the donor impurity binding energies as functions of the impurity position z_i with field strengths of 100 and 300 kV/cm for a QW of $L=100$ Å. Notice the lack in symmetry around the $z_i=0$ position when compared to the binding energy in the absence of an electric field (dashed line). A similar feature is shown in Fig. 1(b), where we display the acceptor impurity binding energies for the same QW as in Fig. 1(a). The external electric field in Figs. 1(a) and 1(b) are in opposite directions, this was done as an aid to the visual comparison of these figures.

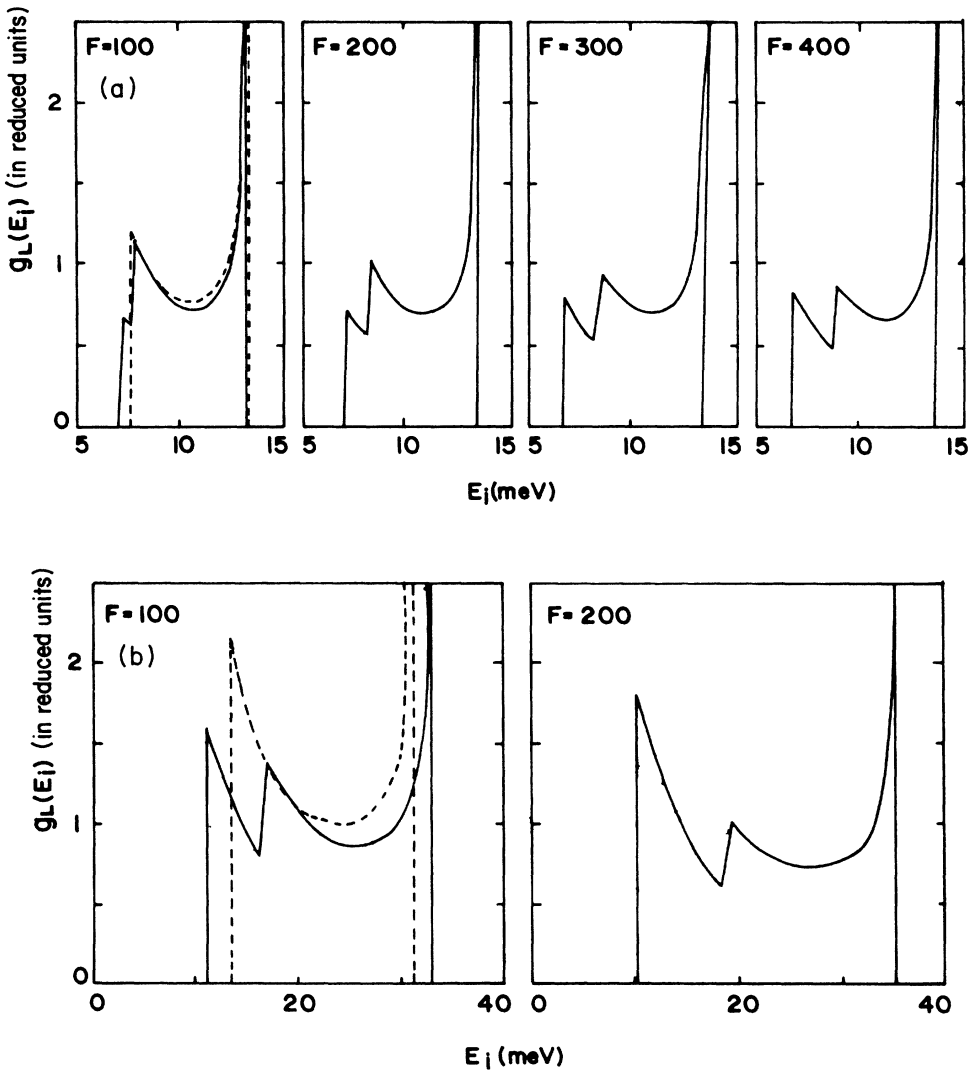

FIG. 2. Densities of (a) donor and (b) acceptor impurity states (in reduced atomic units) as functions of the impurity binding energy, for a QW of $L=100$ Å at several values of the electric-field intensity F (in kV/cm) and in the absence of an electric field (dashed lines).

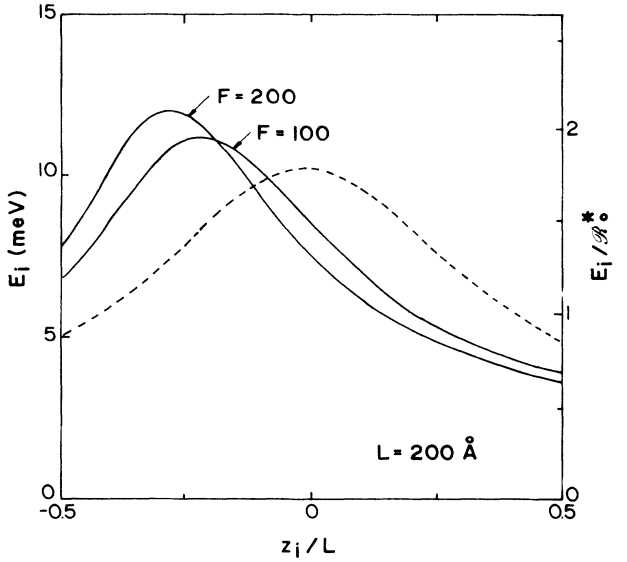

FIG. 3. Binding energies of donors as functions of the impurity position z_i, in a QW with $L=200$ Å, for several values of the electric-field intensity F (in kV/cm) and in the absence of an electric field (dashed lined).

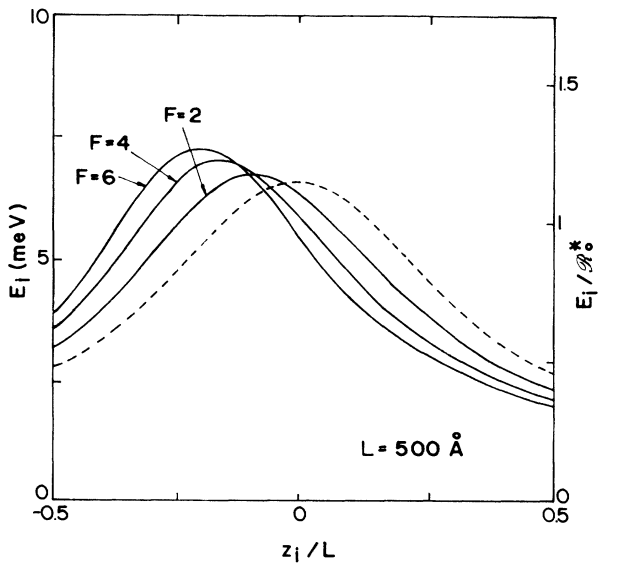

FIG. 4. Binding energies of donors as functions of the impurity position z_i, in a QW with $L=500$ Å, for several values of the electric-field intensity F (in kV/cm) and in the absence of an electric field (dashed line).

The lack in symmetry around the $z_i=0$ position when $F\neq 0$ is reflected in the additional peak in the density of impurity states. In Fig. 2(a) we show the density of donor impurity states and in Fig. 2(b) the density of acceptor impurity states for a QW of $L=100$ Å (the same as in Fig. 1).

When the QW becomes larger, the binding energies become more sensitive to the electric field. This is illustrated in Fig. 3 where we show the donor impurity binding energies for a QW of $L=200$ Å and in Fig. 4 with $L=500$ Å.

The general form of the density of impurity states is not altered substantially when the width of the QW is increased as is it shown in Fig. 5, where we display the den-

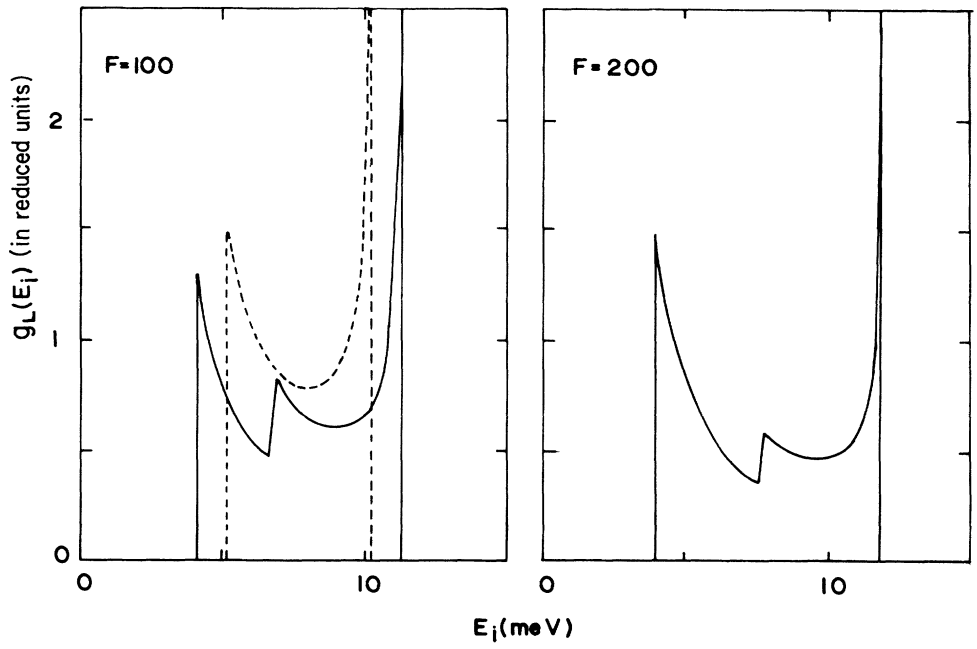

FIG. 5. Density of donor impurity states (in reduced atomic units) as functions of the impurity binding energy, for a QW of $L=200$ Å at several values of the electric-field intensity F (in kV/cm) and in the absence of an electric field (dashed line).

sity of donor impurity states for a QW of $L = 200$ Å.

In Fig. 6(a) we show the total transition probability per unit time, for a QW of $L = 100$ Å, for transitions from the valence-to-donor subbands as functions of $(\hbar\omega - \mathcal{E}_g)$. For a direct comparison with experimental absorption spectra, the energy gap and the $n = 1$ energy levels of the valence and conduction band should be taken into account. Displaying the total transition probability per unit time as function of $(\hbar\omega - \mathcal{E}_g)$ helps the visual inspection of the differences arising due to the electric field. As can be seen in Fig. 6(a), when the electric field increases in intensity, the main high-energy peak (due to impurities at the interfaces) splits into two minor peaks. The low-energy peak (or shoulder) decreases steadily in intensity without modifying its shape. The split of the high-energy level corresponds to the same split seen in Fig. 2(a).

In Fig. 6(b) we display the total transition probability per unit time for a QW of $L = 100$ Å [as in Fig. 6(a)], but now for acceptor-to-conduction subband transitions. As in Fig. 6(a) the split of the high-energy peak occurs but is now hardly visible. This is a feature that could not be predicted by inspecting the density of acceptor impurity states in Fig. 2(b). In Fig. 7 we display the total transition probability per unit time for a QW of $L = 200$ Å for (a) valence-to-donor subband transitions and (b) acceptor-to-conduction subband transitions as functions of $(\hbar\omega - \mathcal{E}_g)$. As previously stated, a larger QW becomes more sensible to the electric field, this is again true in Fig. 7. For valence to donor subband transitions [Fig. 7(a)] we see again the splitting of the high-energy peak (due to

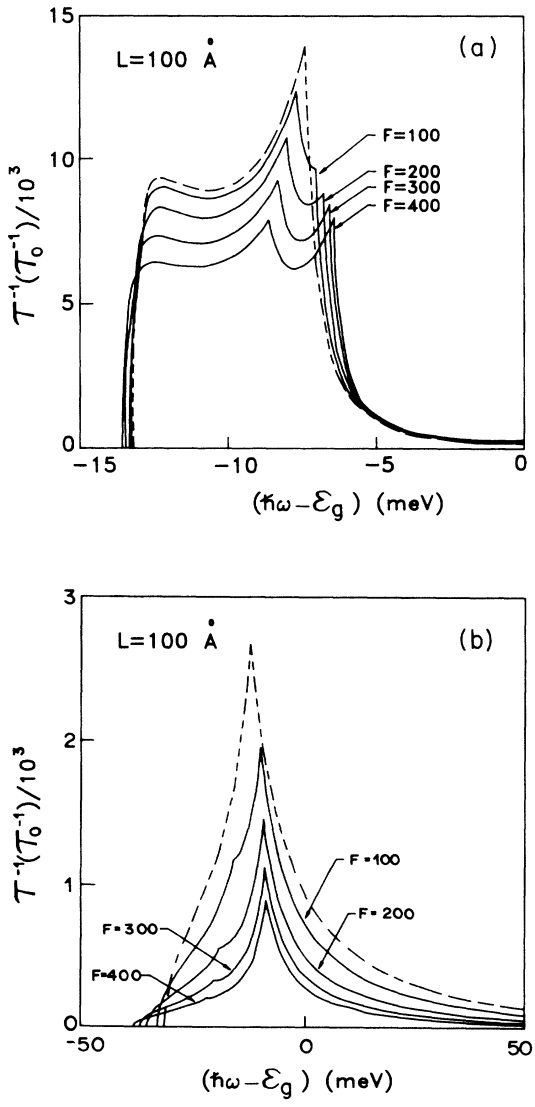

FIG. 6. Total transition probability per unit time (in units of τ_0^{-1}) for (a) valence-to-donor and (b) acceptor-to-conduction subband transitions for a QW of $L = 100$ Å, for several values of the electric-field intensity F (in kV/cm) and in the absence of an electric field (dashed line).

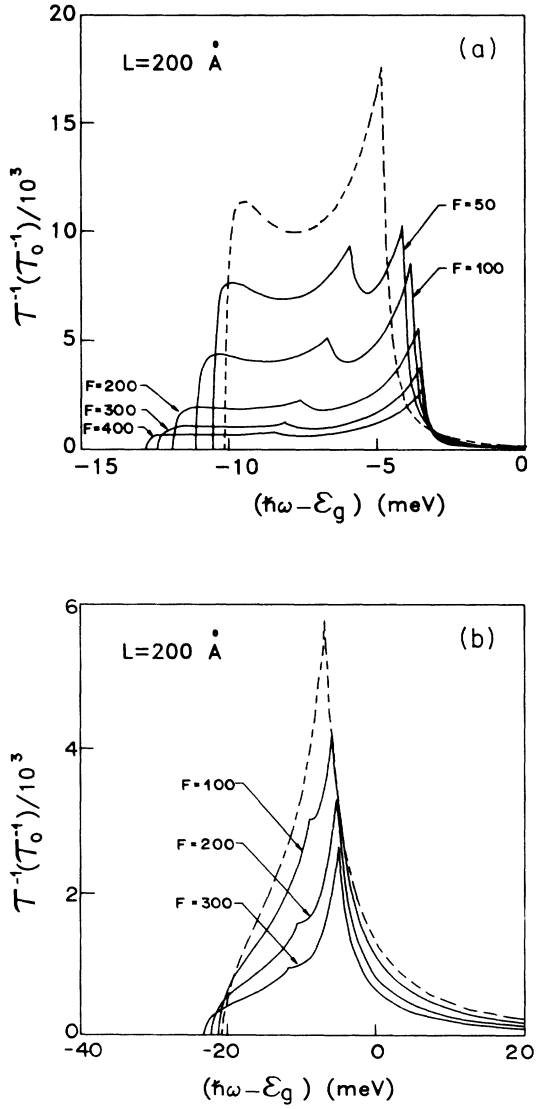

FIG. 7. Total transition probability per unit time (in units of τ_0^{-1}) for (a) valence-to-donor and (b) acceptor-to-conduction subband transitions for a QW of $L = 200$ Å, for several values of the electric-field intensity F (in kV/cm) and in the absence of an electric field (dashed line).

impurities at the well interface), but also we see for high electric fields (400 kV/cm) the almost total quenching of the peak due to impurities at the center interface and with high binding energies, as we saw for acceptors in Fig. 6(b). Figure 7(b) is almost a mere repetition of the features of Fig. 6(b). The effect of the quenching of the peak due to interface impurities with high electric fields can be explained by comparing the effective Bohr radius of the hydrogenic impurity with the well width. When the effective Bohr radius of the hydrogenic impurity is comparable to the well width as in Fig. 6(a), where $a_0^* \simeq 100$ Å and $L = 100$ Å, the peak due to the impurities near the interface and with high binding energy remains strong even at large electric fields. When the effective Bohr radius is smaller than the well width as in fig. 6(b), where $a_0^* \simeq 22$ Å and $L = 100$ Å, this peak is almost totally quenched out. Figs. 7(a) and 7(b) confirm this behavior as we enlarge the well width by a factor of 2.

Comparing our results in the absence of an electric field with those of Oliveira and Pérez-Alvarez[7,8] for infinitely deep QW's, we found quite a good agreement. Our results are numerically somewhat different but this was expected because we are using a different trial impurity wave function and thus obtain a different J function [see Eq. (2.16)]. When we compare our J function with the general expression given by Oliveira and Pérez-Alvarez [Eq. (8) in Ref. 8] we notice that the general J-function behavior is

$$J \sim \frac{2\pi}{\lambda \alpha^3} , \tag{3.1}$$

for infinitely deep QW's multiplied by some slow varying function or even by a constant (for a given β) as it is in our case.

IV. CONCLUSIONS

We calculate the binding energies, densities of impurity states, and total transition probabilities for shallow impurities in QW's of widths ranging typically between 100 and 500 Å.

We show that the quenching of the peak due to interface impurities with high binding energies could not be predicted by a simple inspection of the density of impurity states or the binding energies. This features suggest that experimental and theoretical results concerning shallow impurities in nonintentionally doped QW's should be considered cautiously.

Also we show that our results compare well with previous calculations by Oliveira and Pérez-Alvarez,[7,8] suggesting a general behavior for the J function.

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