Electric-field effects on shallow impurity states in GaAs-(Ga,Al)As quantum wells

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The influence of an applied electric field on shallow donor and acceptor states in GaAs-(Ga,Al)As quantum wells is studied. We work within the effective-mass approximation and adopt a trial envelope wave function for the impurity carrier, which leads to the exact results for vanishing applied electric fields and limiting values of the quantum-well thickness. Results for the binding energies and density of impurity states as functions of the impurity position, well thicknesses, and applied electric field are reported. Some results for the effects of electric field on the donor-related optical properties are also presented. As a general feature, the density of impurity states and impurity-related optical absorption for finite electric fields exhibit three van Hove–like singularities corresponding to the binding energies associated with impurities at the two edges of the quantum well and at the position at which the binding energy has a maximum.

I. INTRODUCTION

The effects of applied electric fields on the physical properties of low-dimensional systems (e.g., inversion layers, quantum wells, superlattices, etc.) constitute a subject of considerable interest both from the theoretical and technological point of view due to the importance of these systems in the development of new semiconductor devices. In particular, the application of an electric field in the growth direction of the heterostructure gives rise to a polarization of the carrier distribution and to an energy shift of the quantum states. Such effects may introduce considerable changes in the energy spectrum of the carriers, which could be used to control and modulate the intensity output of optoelectronic devices.

In the past decade a large number of works devoted to that subject have appeared in the literature. Mendez *et al.*[1] have found that the application of an electric field may induce a semiconductor-semimetal transition in multiple heterostructures. The occurrence of resonant tunneling through one-dimensional double barriers in the presence of an applied electric field (an effect connected with the appearance of negative differential conductivities) has been studied by Ricco and Azbel.[2] Alibert *et al.*[3] with electroreflectance measurements, and Mendez *et al.*[4] and Miller and Gossard[5] with photoluminescence experiments have observed a red shift in the position of the peaks for increasing field strengths in GaAs-(Ga,Al)As quantum wells (QW's). Similar results have been obtained by Wood *et al.*[6] by studying room-temperature excitonic electroabsorption in GaAs-(Ga,Al)As multiple QW's.

The first theoretical attempts in obtaining analytical solutions for the electric-field effects on QW's were made by Fernández and Castro,[7] who considered weak fields and a perturbative approach to calculate the ground-state energy for an infinite GaAs QW with an applied electric field perpendicular to the interfaces, and by Bastard *et al.*,[8] who followed a variational approach for the same problem. Trallero and Gondar[9] obtained the exact wave functions and energy levels for the infinite GaAs QW, whereas Gondar and Enderlein[10] developed a more realistic description of the problem—by considering the finite character of the barriers in their formalism—and studied the electronic density of states and energies of the quasi-bound states. Brum *et al.*[11] were the first to treat the problem of hydrogenic impurities in QW's under the presence of an electric field perpendicular to the interfaces. They reported the field dependence on the binding energy of shallow donors in GaAs-(Ga,Al)As QW's for different well widths and impurity positions.

In the present work we study the influence of an applied electric field on shallow donor and acceptor states in GaAs-(Ga,Al)As QW's. We work within the effective-mass approximation and adopt a trial envelope wave function for the impurity carrier. In Sec. II we present some theoretical aspects of the problem. Results for the binding energy as a function of the impurity position as well as for the density of impurity states are reported in Sec. III. Some results for the impurity-related optical

properties are also presented in Sec. III. We present our conclusions in Sec. IV.

II. THEORY

We consider a finite GaAs-(Ga,Al)As QW described by a parabolic band model in the presence of a constant electric field **F** perpendicular to the interfaces (z direction). The conduction- and valence-band profiles of the QW under consideration are schematically represented in Fig. 1. Tunneling effects due to the presence of the electric field are neglected here. The effective Hamiltonian for a hydrogenic-donor impurity in this system is given by

$$\mathbf{H}=\mathbf{H}_0+V_H(r)\ , \tag{2.1}$$

where

$$\mathbf{H}_0=-(\hbar^2/2)\nabla\cdot[m^*(z)]^{-1}\nabla+V_b\Theta(z^2-L^2/4)+|e|Fz\ , \tag{2.2}$$

and

$$V_H(r)=-\frac{e^2}{\epsilon_0[\rho^2+(z-z_i)^2]^{1/2}}\ . \tag{2.3}$$

The z origin is taken at the center of the well and the energy origin at the bottom of the GaAs conduction band. z_i denotes the impurity position along the growth axis, $r=[\rho^2+(z-z_i)^2]^{1/2}$, with $\rho=(x^2+y^2)^{1/2}$, is the distance from the carrier to the impurity site, and ϵ_0 is the static dielectric constant. V_b is the band offset equal to[12,13] 0.6(0.4) times the band-gap discontinuity ΔE_g (eV)$=1.247x$ for the conduction (valence) band, $m^*(z)$ is the z-dependent effective mass which we considered constant across the interfaces ($m^*=0.0665m_0$ for donors and $m^*=0.30m_0$ for acceptors[14] where m_0 is the free-electron mass), and $\Theta(x)$ is the Heavyside unit-step function. It is important to note that the field **F** appearing in the above equation is the *internal* screened electric field. Also, some of the results presented in this work are given in "reduced atomic units" (a.u.*), which correspond to a length unit of one effective Bohr radius, $a_0^*=\hbar^2\epsilon_0/m^*e^2$, and an energy unit of one effective Rydberg, $R_0^*=m^*e^4/2\hbar^2\epsilon_0^2$. For GaAs-(Ga,Al)As QW's, these units are $a_0^*\simeq 100$ Å and $R_0^*\simeq 5.72$ meV for donors (electrons), and $a_0^*\simeq 22$ Å and $R_0^*\simeq 26$ meV for acceptors (holes).

We focus our attention on the impurity states associated with the QW ground-state subband and assume the trial envelope wave function to be a product of the $\mathbf{H}_0$ ground-state solution and an s-like hydrogenic function which includes the variational parameter λ, i.e.,

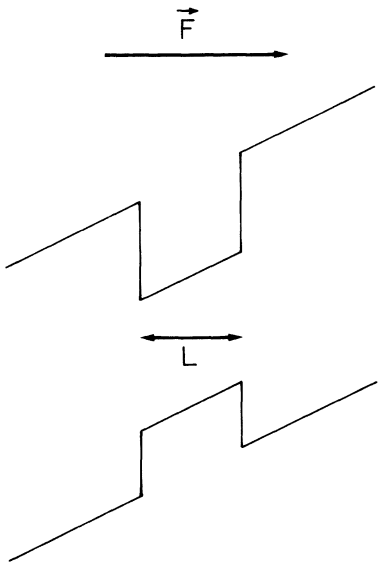

FIG. 1. Conduction- and valance-band profiles corresponding to a GaAs-(Ga,Al)As QW of width L for an electric field **F** applied along the growth direction z.

$$\Psi(\mathbf{r})=N\phi_0(z)\varphi_\lambda(r)\ , \tag{2.4}$$

where N is a normalization constant, $\varphi_\lambda(r)=e^{-r/\lambda}$, and

$$\phi_0(z)=\begin{cases} C_1 e^{k_1(z+L/2)}, & z\le -L/2 \\ \alpha\,\mathrm{Ai}(\xi)+\beta\mathrm{Bi}(\xi), & -L/2\le z\le L/2 \\ C_2 e^{-k_2(z-L/2)}, & z\ge L/2 \end{cases} \tag{2.5}$$

where

$$\mathrm{Ai\ (Bi)}(\xi)=\mathrm{Ai\ (Bi)}(za_c/L-E_0/\hbar\omega_c) \tag{2.6}$$

are the Airy functions[15] and

$$\omega_c=\frac{(eF)^{2/3}}{(2m^*\hbar)^{1/3}}\ , \tag{2.7a}$$

$$a_c=(2m^*\omega_c/\hbar)^{1/2}L\ . \tag{2.7b}$$

In Eq. (2.6), E_0 is the ground-state energy of the QW with the applied field (and without the impurity potential), which is obtained as the first root of the transcendental equation

$$(a_c/L)^2[\mathrm{Ai}'(+)\mathrm{Bi}'(-)-\mathrm{Ai}'(-)\mathrm{Bi}'(+)]+(k_1a_c/L)[\mathrm{Ai}(-)\mathrm{Bi}'(+)-\mathrm{Bi}(-)\mathrm{Ai}'(+)]$$
$$-(k_2a_c/L)[\mathrm{Ai}(+)\mathrm{Bi}'(-)-\mathrm{Ai}'(-)\mathrm{Bi}(+)]-k_1k_2[\mathrm{Ai}(-)\mathrm{Bi}(+)-\mathrm{Ai}(+)\mathrm{Bi}(-)]=0\ , \tag{2.8}$$

where

$$\mathrm{Ai}(\pm)[\mathrm{Bi}(\pm)]=\mathrm{Ai}(\mathrm{Bi})(\pm a_c/2-E_0/\hbar\omega_c)\ , \tag{2.9a}$$

and

$$\mathrm{Ai}'(\mathrm{Bi}')=d\ \mathrm{Ai}(x)[\mathrm{Bi}(x)]/dx\ . \tag{2.9b}$$

The constants in Eq. (2.5) are given by

$$\alpha=[\mathrm{Bi}'(-)a_c/L-k_1\mathrm{Bi}(-)]\ , \tag{2.10a}$$

$$\beta=[k_1\mathrm{Ai}(-)-\mathrm{Ai}'(-)a_c/L]\ , \tag{2.10b}$$

$$C_{1,2}=\alpha\ \mathrm{Ai}(\mp)+\beta\ \mathrm{Bi}(\mp)\ , \tag{2.10c}$$

$$k_{1,2}=[(V_{1,2}-E_0)2m^*/\hbar^2]^{1/2}\ , \tag{2.10d}$$

$$V_{1,2}=V_b\mp|e|FL/2\ . \tag{2.10e}$$

The ground-state energy of a hydrogenic impurity in a GaAs-(Ga,Al)As QW with an applied electric field may be obtained by minimizing

$$\langle\Psi|\mathbf{H}|\Psi\rangle=E_0+\frac{\hbar^2}{2m^*\lambda^2}+\langle\Psi|V_H|\Psi\rangle\ , \tag{2.11}$$

with respect to the variational parameter λ.

The binding energy is therefore given by

$$E_i=E(L,z_i)=-\frac{\hbar^2}{2m^*\lambda_0^2}-\langle\Psi|V_H|\Psi\rangle|_{\lambda_0}\ , \tag{2.12}$$

where λ_0 is the appropriate value of λ which minimizes $\langle\Psi|\mathbf{H}|\Psi\rangle$.

Defining the integrals

$$I_1=\int_{-\infty}^{\infty}dz\phi(z)^2e^{-(2/\lambda_0)|z-z_i|}\ , \tag{2.13a}$$

and

$$I_2=\int_{-\infty}^{\infty}dz\phi(z)^2|z-z_i|e^{-(2/\lambda_0)|z-z_i|}\ , \tag{2.13b}$$

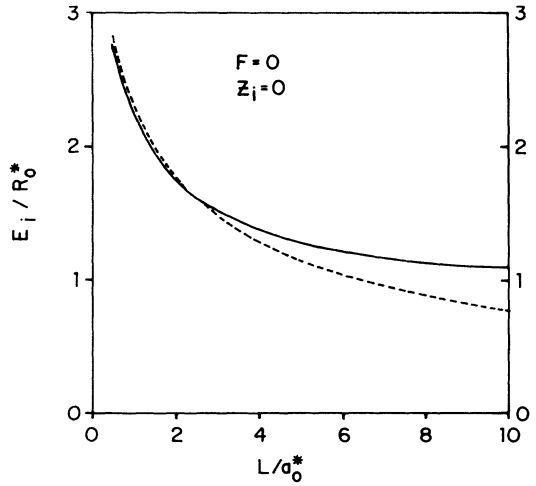

FIG. 2. On-center impurity binding energies for infinite QW's and no applied electric field. Results are presented for the impurity wave function proposed by Brum *et al.* (Ref. 11) (dashed line) and the impurity position-dependent wave function used in this work (solid curve).

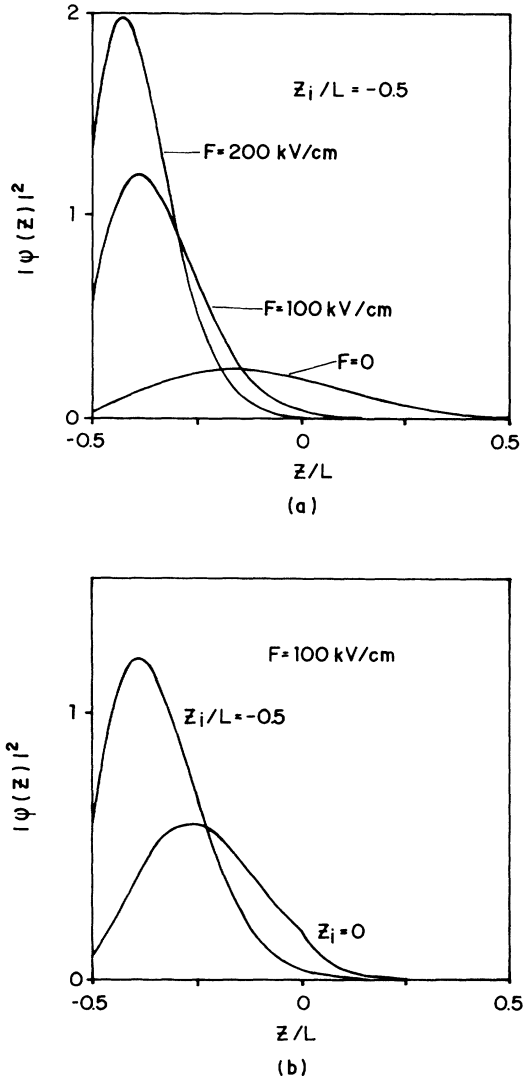

FIG. 3. Probability density $|\Psi(z)|^2$ at $x=y=0$ for a donor state in a GaAs-$Ga_{0.7}Al_{0.3}As$ QW of width $L=200$ Å for (a) impurity located at $z_i=-L/2$ and different electric fields, and (b) impurity located at $z_i=-L/2$ and $z_i=0$ for an electric field of 100 kV/cm.

the contribution of the hydrogenic potential can be written as

$$\langle \Psi | V_H | \Psi \rangle |_{\lambda_0} = -\frac{2e^2}{\epsilon_0} \frac{I_1}{\lambda_0 I_1 + 2I_2} , \tag{2.14}$$

whereas the norm takes the form

$$N = [\pi \lambda_0 (I_2 + \lambda_0 I_1 / 2)]^{-1/2} . \tag{2.15}$$

On the basis of the above equation the impurity binding energies can be evaluated as functions of the impurity position and width of the QW. Also, the density of impurity states, as originally proposed by Bastard,[16] may be readily obtained.

III. RESULTS

Results presented in this section are for both shallow donor and acceptor states. For the latter we use an average spherical effective mass, although a more realistic description should consider the effects of the coupling of the top four valence bands.[17]

The trial envelope wave function we use in the present work explicitly depends on the impurity position z_i and correctly reproduces the results by Bastard[16] in the limit of vanishing electric field (e.g., cf. Fig. 2), in contrast with what one would obtain by using the z_i independent trial function proposed by Brum *et al.*[11] (the dependence of

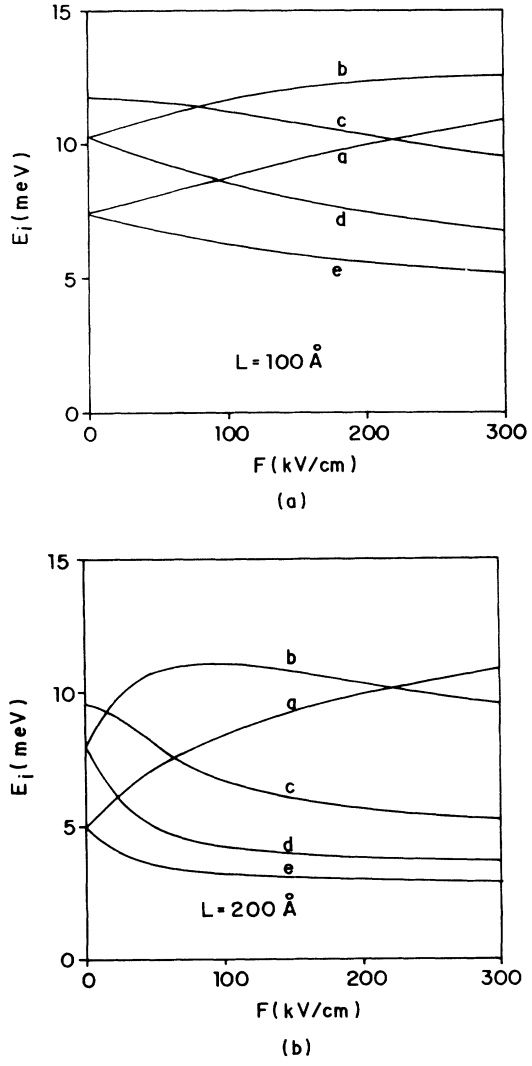

FIG. 4. Impurity binding energies as functions of the applied electric field for a GaAs-$Ga_{0.7}Al_{0.3}As$ QW of thickness (a) $L = 100$ Å and (b) $L = 200$ Å for five different positions of the donor impurity, i.e., *a*, $z_i = -L/2$; *b*, $z_i = -L/4$; *c*, $z_i = 0$; *d*, $z_i = L/4$; *e*, $z_i = L/2$.

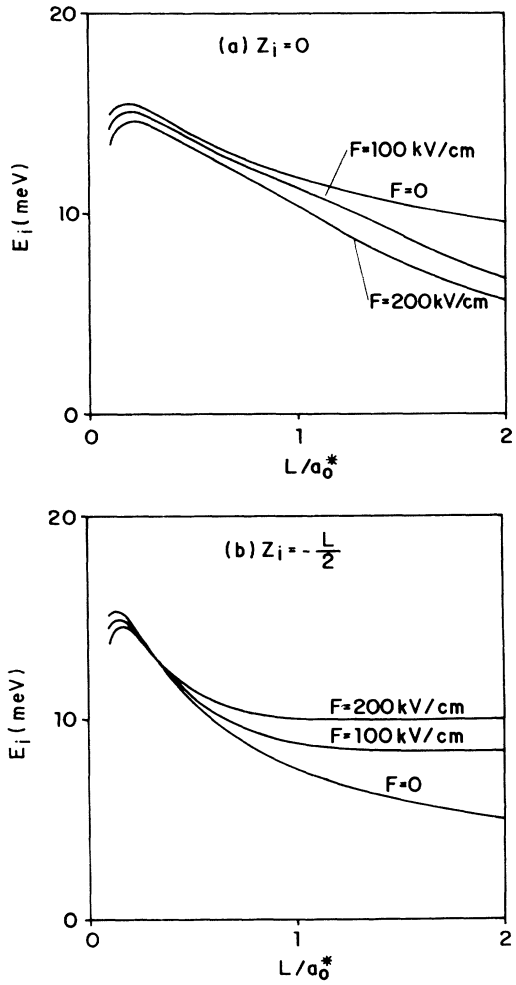

FIG. 5. Donor binding energies for a GaAs-$Ga_{0.7}Al_{0.3}As$ QW as functions of the well thickness for (a) $z_i = 0$ (on-center position), and (b) $z_i = -L/2$ (on-edge position) and different values of applied electric field.

their envelope wave function on the impurity position comes via the variational parameter λ through the z_i dependence of the Hamiltonian). In particular, for $z_i = 0$ and in the $L \to \infty$ limit, our choice for the impurity envelope wave function gives the exact bulk results $E_i / R_0^* = 1$. This provides an indication that our choice for the variational envelope wave function (with an explicit dependence on the impurity position z_i) is more realistic than the one used by Brum *et al.*[11]

Figure 3 shows the density of probability distribution $|\Psi(z)|^2$ inside a $L = 200$ Å well for $\rho = 0$ in the case of a donor impurity at $z_i = -L/2$ for three different field strengths (0, 100, and 200 kV/cm), and in the case of an on-center impurity for $F = 100$ kV/cm. It can be clearly seen that the electric field tends to concentrate the electronic charge on one of the sides of the QW (cf. Fig. 1). Depending on the position of the impurity inside the well, such an effect may either increase or reduce the binding energy. For $z_i = -L/2$ the increase of the field strength clearly leads to an enhancement of E_i due to the increased charge concentration around the impurity site. On the other hand, for on-center impurities, as the field increases one observes a reduction of the binding energy as a consequence of the displacement of the electronic charge with respect to the impurity position. The dependence of the donor binding energy with the applied electric field for $L = 100$ Å and $L = 200$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW's is shown in Fig. 4 for different donor positions. Also, the dependence of the binding energies of on-center and on-edge donor impurities on the well

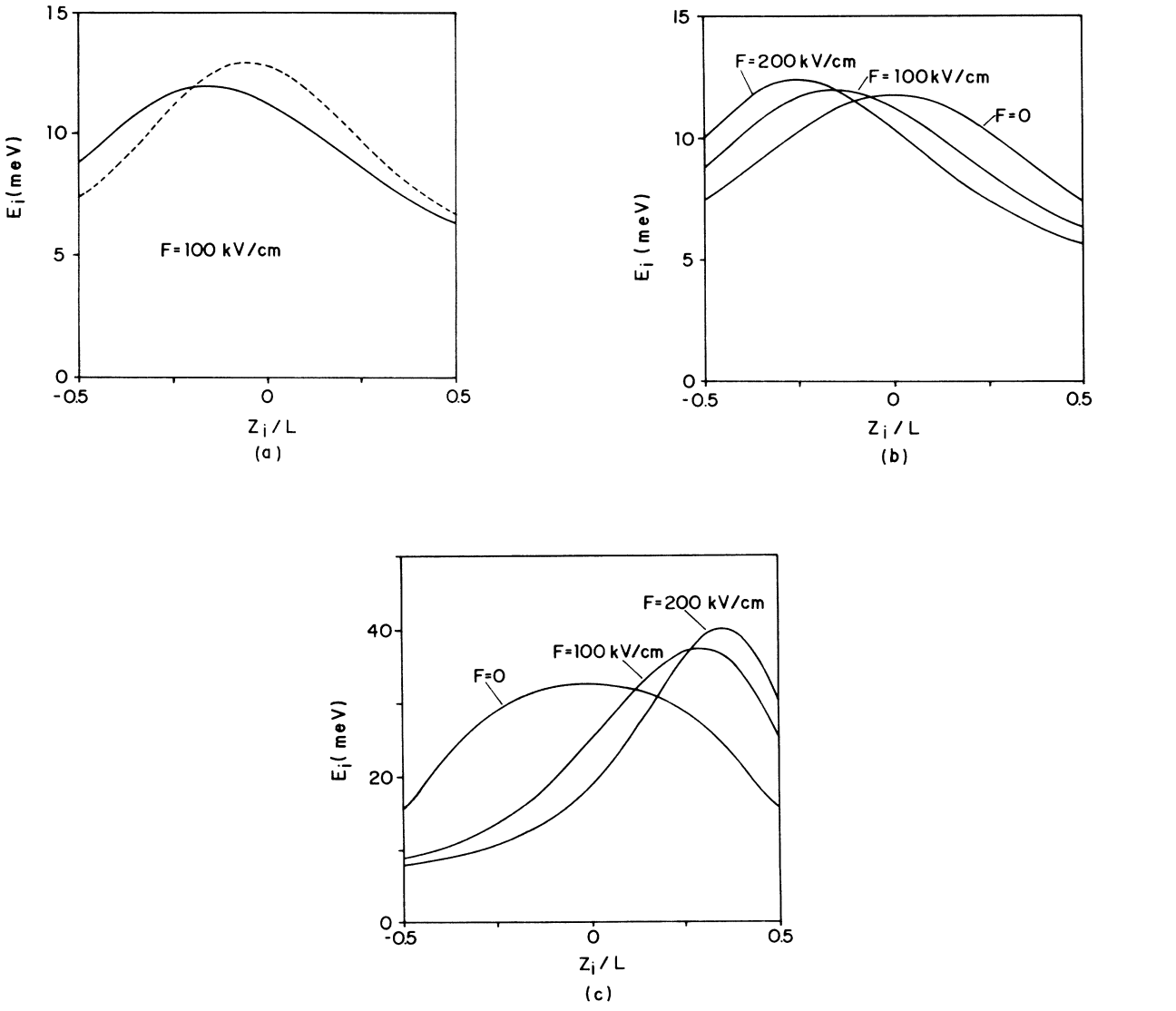

FIG. 6. Impurity binding energies for a GaAs-$Ga_{0.7}Al_{0.3}As$ QW with thickness $L = 100$ Å as functions of the impurity positions in the case of (a) donor states with an applied electric field of 100 kV/cm (dashed line corresponds to an infinite well), (b) donor states for different applied electric fields, and (c) acceptor states for different applied electric fields.

thickness is shown in Fig. 5 for $F=0$, 100, and 200 kV/cm. Results by Brum *et al.*,[11] who considered a different barrier potential and used a z_i independent variational wave function, are in qualitative agreement with ours.

The importance of considering a finite band offset as compared with an infinite barrier GaAS QW is illustrated in Fig. 6(a) for Al concentration $x=0.3$, $L=100$ Å, and $F=100$ kV/cm. The behavior of donor and acceptor binding energies as functions of the impurity position and of increasing electric field applied along the positive z direction for a $L=100$ Å GaAs-$Ga_{0.7}Al_{0.3}As$ QW is also shown in Figs. 6(b) and 6(c), respectively. For donors at $z_i=-L/2$ ($z_i=L/2$), the binding energy increases (decreases) with the field strength due to the larger (smaller) concentration of the electronic charge around the impurity site caused by the "triangular" QW. For acceptors, the same situation occurs at $z_i=+L/2$ ($z_i=-L/2$) because of the positive charge of the hole. The results for an infinite QW obtained by Weber[18]—who has used a less accurate and z_i independent trial wave function for the impurity ground state—agree only qualitatively with our calculations.

From the knowledge of the binding energy as a function of the impurity position and of the probability distribution of impurities in the well one may calculate the density of impurity states[14,16,18] $g_L(E_i)$ per unit of binding energy. Assuming a homogeneous distribution of noninteracting impurities inside the GaAs well, we have evaluated the density of impurity states for GaAs-

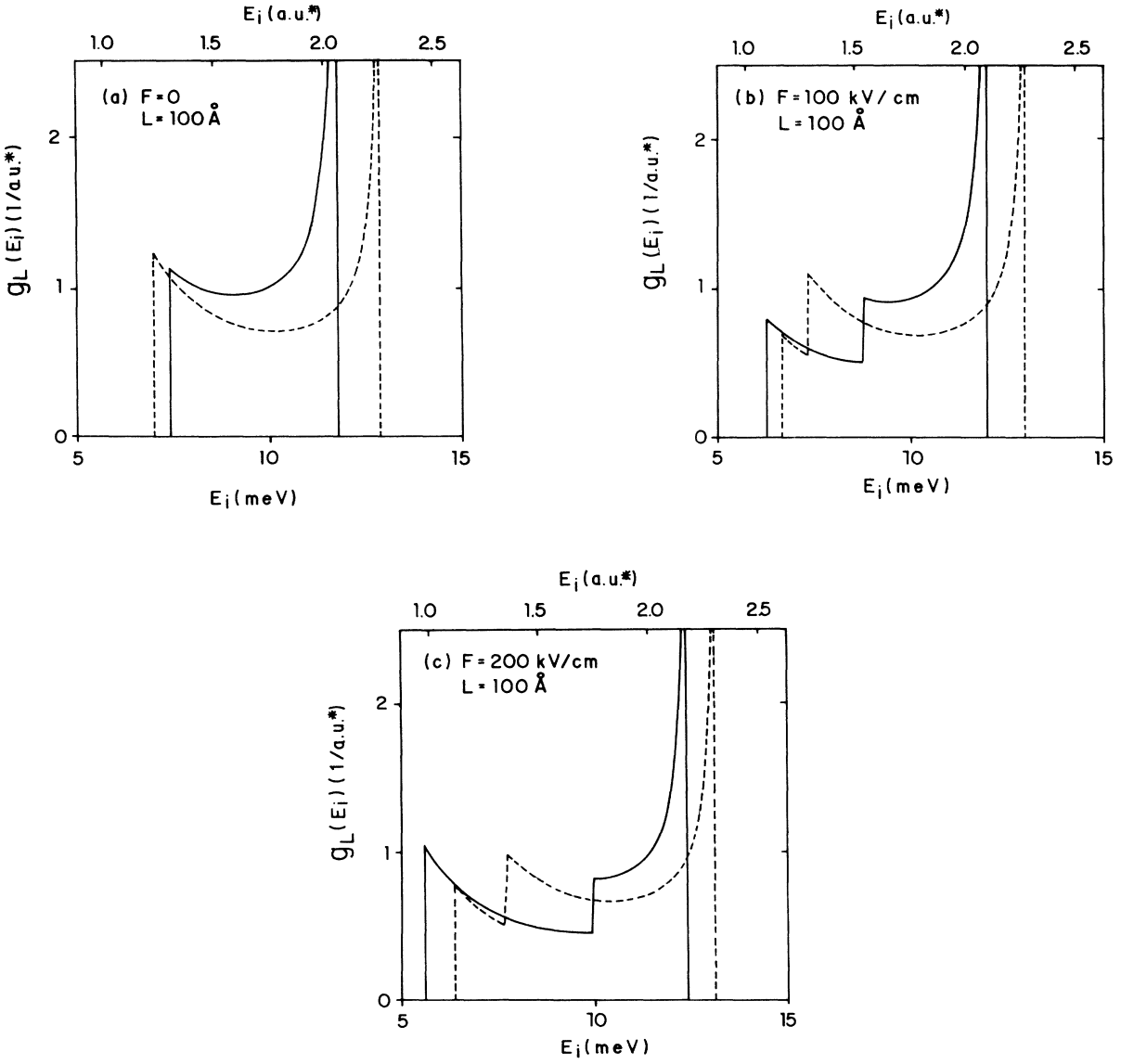

FIG. 7. Densities of donor states in reduced atomic units as functions of the impurity binding energy $E_i=E(L,z_i)$ for various applied electric fields. Dashed curves are for infinite QW's whereas solid curves correspond to a GaAs-$Ga_{0.7}Al_{0.3}As$ QW of thickness $L=100$ Å.

$Ga_{0.7}Al_{0.3}As$ QW's of different thicknesses and for increasing applied electric fields. Results for shallow donors are shown in Fig. 7—together with those for an infinite GaAs QW—and Fig. 8. Calculations for shallow acceptor states are presented in Fig. 9. In the case of $F=0$ [Fig. 7(a)], it is clear that the width of the impurity band is reduced when the finite character of the band offset is taken into account. As a general feature, the density of impurity states for finite F exhibits three van Hove-like structures corresponding to the binding energies associated with impurities at $z_i=L/2$, $-L/2$, and z_m, where z_m is the position at which E_i has a maximum (cf. Fig. 6). Of course, these van Hove-like structures will show up as features corresponding to special transitions in the impurity-related absorption and photoluminescence spectra.[19,20] This is clearly seen in Fig. 10, which shows the absorption[19] spectra for $F\rightarrow 0$ and $F=200$ kV/cm in the case of a $L=100$ Å GaAs-$Ga_{0.3}Al_{0.7}As$ QW corresponding to transitions from the $n=1$ valence subband to the donor impurity band. In the limit of vanishing applied electric field, we recover the results for the impurity-related optical properties first obtained by Oliveira and Pérez-Alvarez.[19] For the case of an infinite barrier, the results obtained by Weber[18] for the impurity-related optical absorption do not present the proper zero-field limit.[19] We believe this is due to the choice of a less accurate impurity envelope wave function. A detailed theoretical study of electric-field effects on the

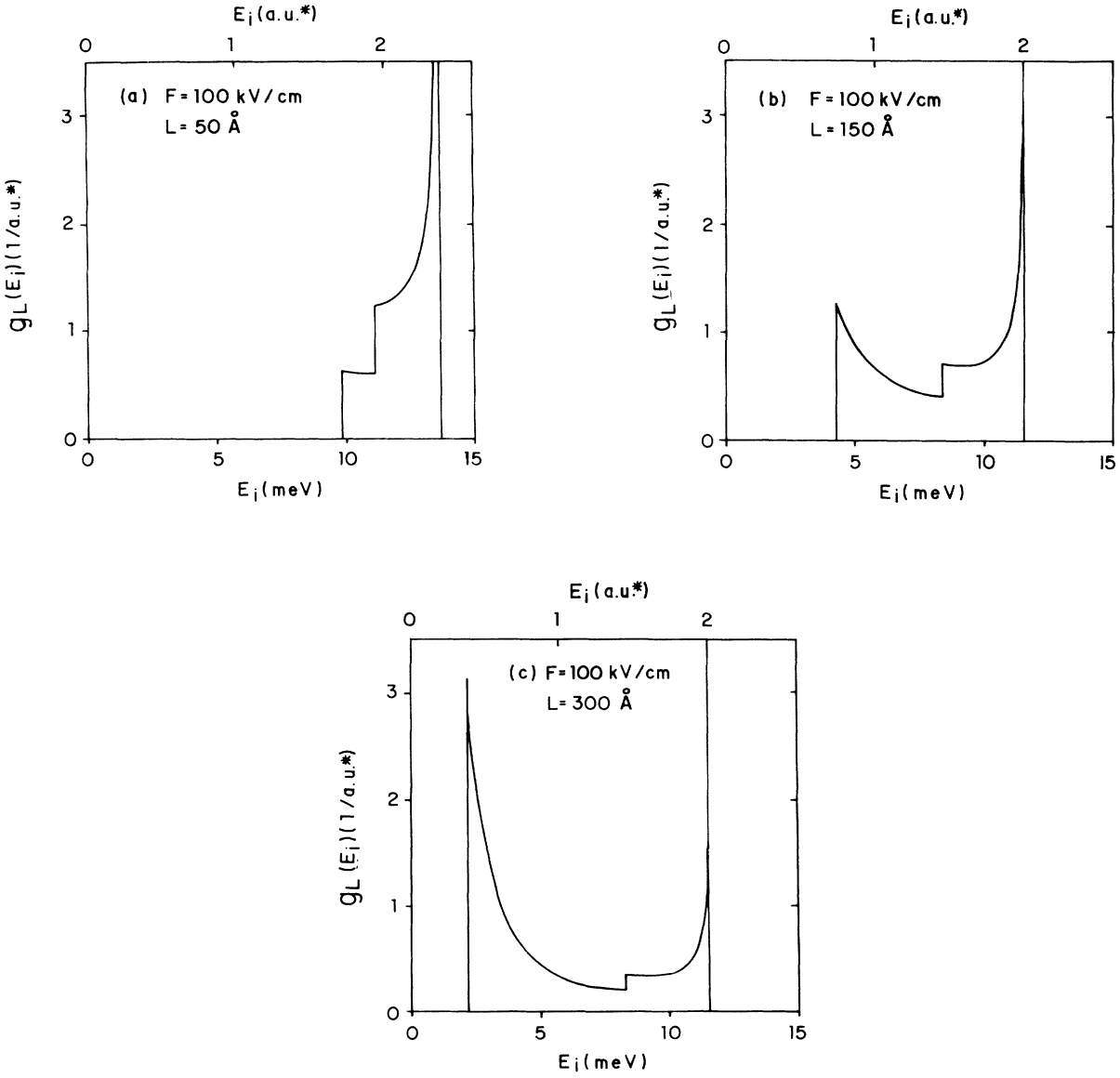

FIG. 8. Densities of donor states in reduced atomic units as functions of the impurity binding energy $E_i=E(L,z_i)$, for a fixed electric field $F=100$ kV/cm, and for various GaAs-$Ga_{0.7}Al_{0.3}As$ QW thicknesses.

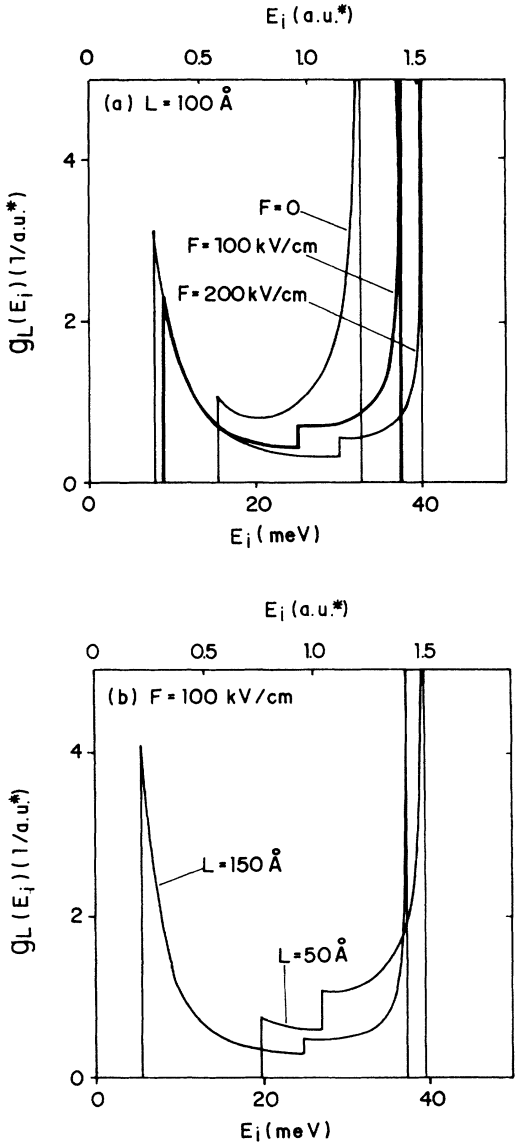

FIG. 9. Densities of acceptor states in reduced atomic units as functions of the impurity binding energy for GaAs-$Ga_{0.7}Al_{0.3}As$ QW's; (a) $L=100$ Å and various applied electric fields; (b) electric field $F=100$ kV/cm and two different QW thicknesses.

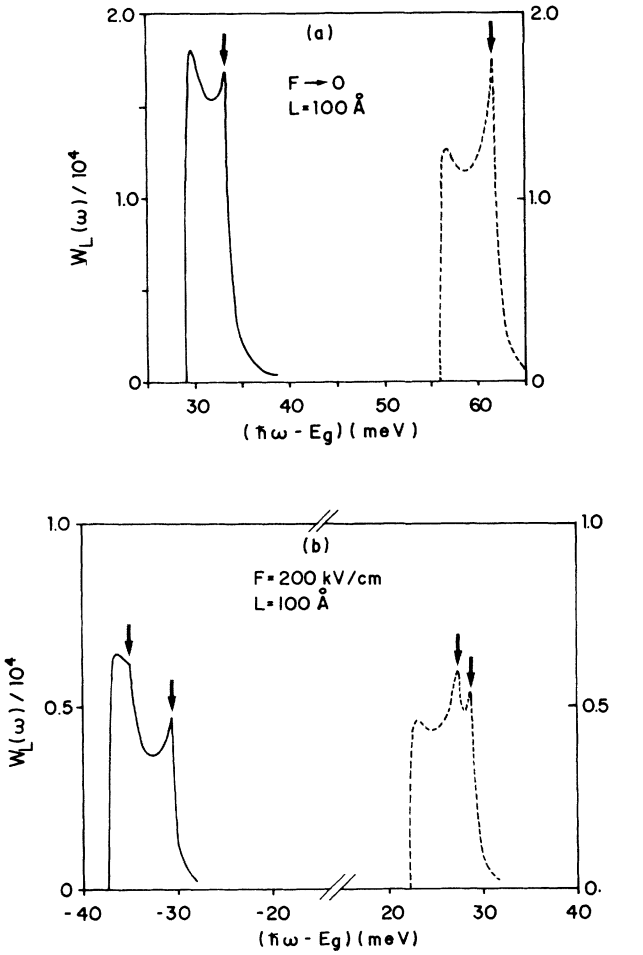

FIG. 10. Absorption spectra for valence to donor transitions (in units of W_0; see text) for GaAs-(Ga,Al)As QW's of width $L=100$ Å and electric fields $F=0$ and $F=200$ kV/cm. Dashed lines correspond to infinite depth QW's, whereas solid curves indicate a $x=0.30$ Al concentration (finite barrier potential). The arrows signal the van Hove-like structures corresponding to transitions associated with $z_i=\pm L/2$. Notice that different scales are used.

donor- and acceptor-related optical absorption and photoluminescence properties in GaAs-(Ga,Al)As QW's is in progress and will be presented elsewhere.

IV. CONCLUSIONS

In this work we present results for the binding energies of shallow donor and acceptor states in GaAs-(Ga,Al)As QW's under the influence of an applied electric field. We work within the effective-mass approximation and we use a trial envelope wave function for the impurity carrier which leads to the exact results for vanishing applied electric fields and limiting values of the quantum-well thickness. We thoroughly investigate the dependence of both the binding energies and density of impurity states as functions of the impurity position, well thicknesses, and applied electric field. Results by Brum, Priester, and Allan[11] and Weber[18] for the impurity binding energies are in qualitative agreement with our calculations, which are based on a more realistic description of the impurity envelope wave function. Some results for the effects of electric field on the donor-related optical properties are also presented for both infinite and finite GaAs-(Ga,Al)As QW's. As a general feature, the density of impurity states and impurity-related optical absorption for finite electric fields exhibit three van Hove-like singularities corresponding to the binding energies associated with impurities at the two edges of the quantum well and at the position at which the binding energy has a maximum.

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