Impurity-related optical absorption from GaAs-(Ga,Al)As quantum wells under an applied electric field

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Impurity-related optical-absorption spectra for GaAs-(Ga,Al)As quantum wells under an externally applied longitudinal electric field are investigated. A variational procedure in the effective-mass approximation is used in the evaluation of the impurity binding energies and wave functions. Effects of the variation of both field intensity and well width on the donor- and acceptor-related absorption line shapes are analyzed in the cases of infinite- and finite-barrier potentials. The results show that the absorption spectra present an edge associated with the maximum value of the impurity binding energy and two van Hove–like singularities corresponding to impurities positioned at the two edges of the well. As the field intensity is increased, the absorption spectra are shifted towards lower energies, with their intensities reduced, and the relative importance of the van Hove–like singularities is changed. Such effects become more pronounced for larger widths of the quantum wells.

I. INTRODUCTION

The understanding of the electronic and impurity properties of semiconducting heterostructures such as quantum wells (QW's), quantum-well wires (QWW's), and quantum dots (QD's) is a problem of considerable importance from both basic and technological points of view. Special interest has been focused on GaAs-$Ga_{1-x}Al_xAs$ heterostructures, which exhibit a direct band gap for Al concentration x below 0.40–0.45. Bastard[1] studied the problem of hydrogenic impurities in infinite-barrier QW's, by analyzing the binding energy, the density of impurity states, and the optical and photoluminescence spectra of shallow donors and acceptors. The finite band offset in GaAs-(Ga,Al)As QW's was discussed independently by Mailhiot, Chang, and McGill[2] and Greene and Bajaj.[3] Mailhiot, Chang, and McGill[2] and Fraizzoli, Bassani, and Buczko[4] have considered the role of the effective-mass and dielectric-constant mismatches across the interfaces of the QW on the impurity problem. Effects of nonparabolicity of the conduction band were taken into account by Chaudhuri and Bajaj,[5] the complex structure of the valence band in the case of acceptors was considered by Masselink, Chang, and Morkoç,[6] and spatially dependent screening effects were studied by Csavinszky and Elabsy[7] and Oliveira and Falicov.[8]

On the experimental ground, significant progress has been made regarding the preparation and characterization of the physical properties of semiconducting heterostructures. Donor and acceptor features[9] have been observed in photoluminescence experiments in doped GaAs-(Ga,Al)As QW's. Recent reviews[10] present a detailed account of experimental and theoretical work concerned with shallow impurities in QW's.

The application of an external electric field can lead to significant changes in the physical properties of semiconducting materials. In particular, for an applied electric field along the heterostructure growth direction, polarization of the carrier distribution and shifts of the quantum states of the system may be of importance for control and modulation of intensity outputs of optoelectronic devices. Brum, Priester, and Allan,[11] Weber,[12] and López-Gondar, d'Albuquerque e Castro, and Oliveira[13] theoretically studied the effects of an external electric field on the binding energies and density of impurity states associated with shallow donors and acceptors in GaAs-(Ga,Al)As QW's.

In the present work we are concerned with the investigation of the optical-absorption spectra associated with shallow impurities in GaAs-(Ga,Al)As QW's subjected to an externally applied electric field. We organize the paper as follows. In Sec. II we briefly outline the theory regarding the impurity-related optical absorption. Results and discussion are presented in Sec. III, and our conclusions are in Sec. IV.

II. THEORY

Within the effective-mass approximation and the parabolic-band model, the Hamiltonian for a shallow hydrogenic impurity in a GaAs-(Ga,Al)As QW, subjected to a constant electric field F perpendicular to the interfaces (z direction), is given by

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$$H=-(\hbar^2/2m^*)\nabla^2-\frac{e^2}{\kappa[\rho^2+(z-z_i)^2]^{1/2}}+V_b\Theta(z^2-L^2/4)+|e|Fz\ . \quad (2.1)$$

The z origin is taken at the center of the well and the energy origin at the bottom of the GaAs conduction band. The impurity position along the growth axis is denoted by z_i, and $r=[\rho^2+(z-z_i)^2]^{1/2}$, with $\rho=(x^2+y^2)^{1/2}$, is the distance from the carrier to the impurity site. V_b is the band offset equal to[14,15] 0.6 (0.4) times the band-gap discontinuity[16] $\Delta E_g=1.247x$ eV for the conduction (valence) band, m^* is the effective mass which we consider constant across the interfaces ($m_c^*=0.0665m_0$ for donors and $m_v^*=0.33m_0$ for acceptors,[8] where m_0 is the free-electron mass), and $\Theta(z)$ is the Heaviside unit-step function. We neglect the mismatch of the dielectric constant of the two materials and assume that $\kappa=13.1$ (Ref. 17). One should note that the field F appearing in Eq. (2.1) is the *internal* screened electric field. We neglect tunneling effects due to the presence of the electric field. Some of the results presented in this work are given in effective[13] "reduced units" (a.u.*).

The ground-state wave function and energy of the above Hamiltonian can be obtained approximately using a variational procedure. A convenient choice for the trial envelope wave function ψ is given[13] by the normalized product of the ground-state wave function $\phi_0^{c,v}(z)$ for the QW in the absence of the impurity [upper indices (c,v) refer to conduction and valence subbands] and a hydrogenic s-wave function $\exp[-\lambda r]$, in which λ is taken as the variational parameter. The optimal value of λ is determined by minimizing the expectation value $\langle\psi|H|\psi\rangle$. The binding energy of the impurity is then defined as

$$E_i=E(L,z_i)=E_0-\langle\psi|H|\psi\rangle\ , \quad (2.2)$$

where E_0 is the ground-state energy of the QW in the presence of the applied electric field and without the impurity, which is given by the lowest root of the transcendental equation[18] (2.8) in López-Gondar, d'Albuquerque e Castro, and Oliveira.[13]

We are interested in calculating the transition probability per unit time $W_L(z_i,\omega)$ for valence to donor transitions (associated to a single impurity located at $z=z_i$), which can be obtained[19] from the matrix element of the electron-photon interaction H_{int} between the wave functions of the initial ($n=1$ valence subband) and final (impurity) states, with $H_{\text{int}}=C\mathbf{e}\cdot\mathbf{p}$, where $\mathbf{e}$ is the polarization vector in the direction of the electric field of the radiation, $\mathbf{p}$ is the momentum operator, and C is a prefactor which contains the photon vector potential. Therefore, for a GaAs-(Ga,Al)As QW of width L, we can write[20,21]

$$W_L(z_i,\omega)=W_0\frac{1}{2}\frac{m_v^*}{m_0}\frac{1}{a_0^2}S^2(z_i,\lambda,k_\perp(\omega))\Theta(\Delta), \quad (2.3)$$

where a_0 is the Bohr radius, and

$$\Delta=\hbar\omega-\varepsilon_g+E(L,z_i)\ , \quad (2.4a)$$

$$k_\perp(\omega)=(2m_v^*\Delta/\hbar^2)^{1/2}\ , \quad (2.4b)$$

$$\varepsilon_g=E_g+E_{n=1}^c+E_{n=1}^v\ , \quad (2.4c)$$

$$W_0=\frac{4m_0}{\hbar^3}a_0^2|C|^2|\mathbf{e}\cdot\mathbf{P}_{fi}|^2\ . \quad (2.4d)$$

In the above equations, E_g is the bulk GaAs gap, $E_{n=1}^c$ ($E_{n=1}^v$) is the bottom (top) of the first conduction (valence) subband [cf. Fig. 1 of Ref. 20], $\mathbf{P}_{fi}$ is a matrix element of the momentum operator,[20] and $S(z_i,\lambda,k_\perp(\omega))$ is given by

$$S(z_i,\lambda,k_\perp(\omega))=\frac{2\pi N_i^cN_v}{\beta^3\lambda}\int_{-\infty}^{\infty}dz[1+\beta|z-z_i|]\phi_0^c(z)\times\phi_0^v(z)e^{-\beta|z-z_i|}\ , \quad (2.5)$$

with

$$\beta=\beta(k_\perp)=(k_\perp^2+\lambda^{-2})^{1/2}\ , \quad (2.6)$$

and N_i^c and N_v are the normalization factors for the donor envelope wave function and the first valence subband, respectively.

Finally, one has for the total number of transitions per unit of time per unit of volume

$$W_L(\omega)=\frac{1}{L}\int_{-L/2}^{L/2}dz_in_d(z_i)W_L(z_i,\omega)\ , \quad (2.7)$$

where $n_d(z_i)$ is the density of donor impurities per unit of volume. In this work, we assume a homogeneous distribution of impurities inside the QW, i.e., $n_d(z_i)=1$.

The case of transitions from an acceptor impurity band to the first conduction subband is obtained by performing the change $m_v^*\leftrightarrow m_c^*$—and by exchanging the barrier potentials associated to the valence and conduction subbands— through Eqs. (2.2)–(2.7).

III. RESULTS AND DISCUSSION

We present in this section the results of the optical line shape associated to impurities in GaAs-$Ga_{1-x}Al_xAs$ QW's. Our calculations were performed for $x=0.3$ and we have considered both cases of absorption from the $n=1$ valence subband to the donor-impurity band and from the acceptor band to the $n=1$ conduction subband. We have assumed that the temperature is much higher than the impurity binding energies so that the impurity states are ionized. Further, we have assumed a simple parabolic band to describe the valence (and acceptor) states, although a realistic description would consider effects of the coupling of the top four valence bands.[6] Our results are for different QW widths and electric-field intensities. In addition, we have made comparison with predictions based on an infinite well barrier model.

The optical absorption associated with transitions involving donor states is presented in Fig. 1 for an $L=100$ Å QW and for different values of the applied electric field. A comparison between the optical line shapes corresponding to the infinite- and finite-barrier potentials is shown. For zero field, our results are in agreement with

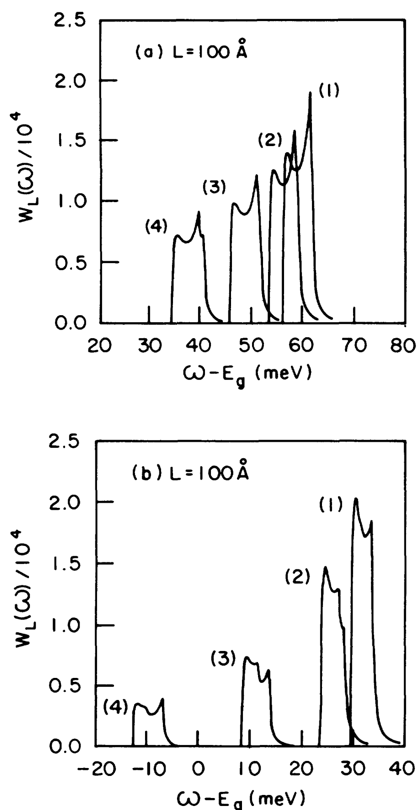

FIG. 1. Donor-related optical-absorption spectra (in units of W_0; see text) under applied electric field for GaAs-$Ga_{0.7}Al_{0.3}As$ QW's of width $L = 100$ Å. Results are presented for infinite- (a) and finite- (b) barrier potentials, and for electric fields of (1) zero, (2) 50 kV/cm, (3) 100 kV/cm, and (4) 150 kV/cm.

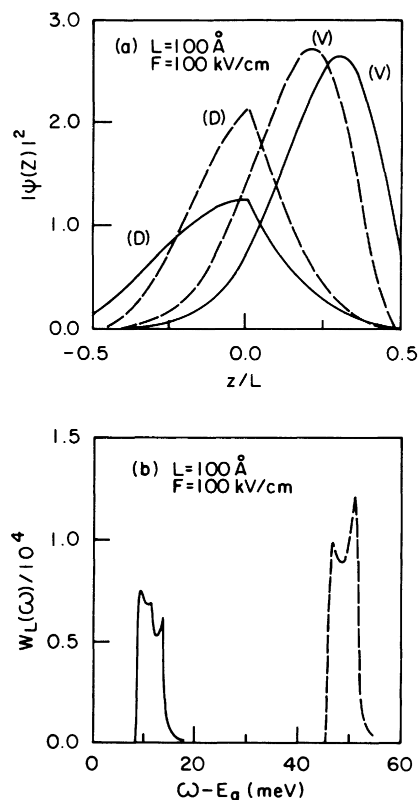

FIG. 2. (a) Probability density corresponding to effective-mass envelope wave functions $\psi(x=0,y=0,z)$ for $n=1$ valence states (V) and on-center donor states (D); (b) absorption spectra (in units of W_0; see text) for valence to donor transitions. Results are presented for GaAs-$Ga_{0.7}Al_{0.3}As$ QW's of width $L = 100$ Å and for $F = 100$ kV/cm, and for infinite- (dashed lines) and finite- (solid curves) barrier potentials.

those of Oliveira and Pérez-Alvarez.[20,22] We note that the effect of the application of the electric field is to introduce a redshift in the spectra and a reduction in the absorption intensity. One clearly notices that such an effect is more pronounced in the case of finite barriers. For a given applied electric field, the main features of the spectrum are the presence of van Hove–like singularities associated with transitions involving donors at QW positions corresponding to the maximum value of the impurity binding energy (lower edge of the spectrum) and with transitions to donor states related to impurities at the edges of the QW. These features are most clearly seen in the case of a finite barrier and $F = 100$ kV/cm [cf. solid curve in Fig. 2(b)]. The redshift in the absorption spectra is essentially due to the reduction in the energy difference between the first valence and donor states in the QW, caused by the application of the electric field which gradually transforms the rectangular QW into a triangular-shaped QW. The reduction in the absorption intensity with increasing electric field comes from the reduction in the overlap between donor- and valence-state wave functions, as can be clearly seen in Fig. 2(a), which depicts the probability density for on-center donor and valence states for $F = 100$ kV/cm. Such a reduction in the overlap is more pronounced in the case of finite potentials because the impurity and valence wave functions are allowed to penetrate into the barrier.

The donor-related optical-absorption line shapes for $L = 50$ and 200 Å GaAs-(Ga,Al)As QW's are shown in Figs. 3 and 4, respectively, for different values of applied electric fields. We can observe that, for a fixed value of the electric field, the redshift in the energy position of the spectra becomes more pronounced as the width of the well increases, as expected. Also the splitting in energy of the two van Hove–like structures associated to impurities at the two opposite edges of the QW becomes more pronounced with increasing field and/or increasing QW width. For an $L = 200$ Å QW and electric fields larger than approximately 100 kV/cm, one notices a dramatic decrease in the absorption intensity, which is due to the strong reduction in the overlap between the donor- and valence-state wave functions, as depicted in Fig. 5 for on-center donor states.

In Fig. 6 we show the absorption spectra for valence to donor transitions for infinite and finite QW's of width $L = 100$ Å and electric field $F = 200$ kV/cm. As discussed above, the absorption intensity in the case of a finite barrier is much smaller than in the case of an infinite potential, contrary to what is presented in Fig.

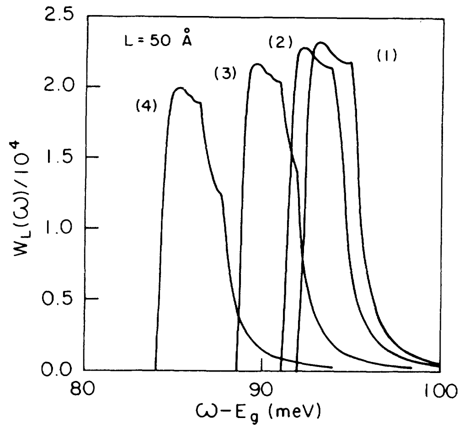

FIG. 3. Donor-related optical-absorption spectra (in units of W_0; see text) under applied electric field for a GaAs-$Ga_{0.7}Al_{0.3}As$ QW of width $L = 50$ Å. Results are presented for electric fields of (1) zero, (2) 50 kV/cm, (3) 100 kV/cm, and (4) 150 kV/cm.

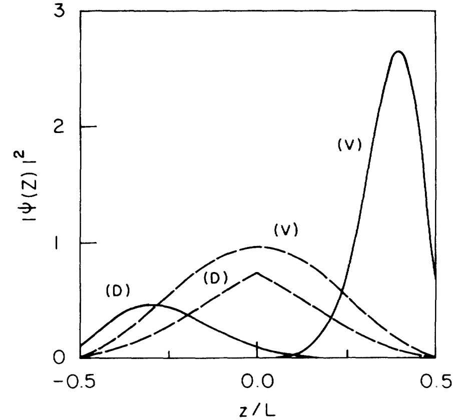

FIG. 5. Probability density corresponding to effective-mass envelope wave functions $\psi(x=0,y=0,z)$ for $n=1$ valence states (V) and on-center donor states (D), for a GaAs-$Ga_{0.7}Al_{0.3}As$ QW of width $L = 200$ Å, and applied electric field $F=0$ (dashed lines) and 100 kV/cm (solid curves).

10(b) of López-Gondar, d'Albuquerque e Castro, and Oliveira.[13]

The absorption line shapes for the case of transitions from the acceptor impurity band to the first conduction subband are shown in Figs. 7 and 8(c), for the case of infinite and finite $L = 100$ Å QW's, respectively, and for different applied electric fields. In the case of an infinite potential barrier, our results are in qualitative agreement with those of Weber,[12] although his choice for the impurity envelope wave function leads to a less accurate description of the absorption line shape. On comparing our results for infinite barriers with those for the finite ones, we clearly see that the acceptor-related optical line shapes are sharper in the latter cases. In addition, we find that the dependence of the absorption intensity with the applied electric field is quite distinct in the cases of infinite and finite barriers, and that the van Hove–like singularity associated with transitions involving $z_i = -L/2$ acceptor states becomes hardly noticeable in both cases. Such a behavior may be understood from the analysis of the binding-energy curves as a function of the acceptor position in the QW and for different applied electric fields [cf. Fig. 8(a)]. The absorption intensity is basically determined by the joint density of states be-

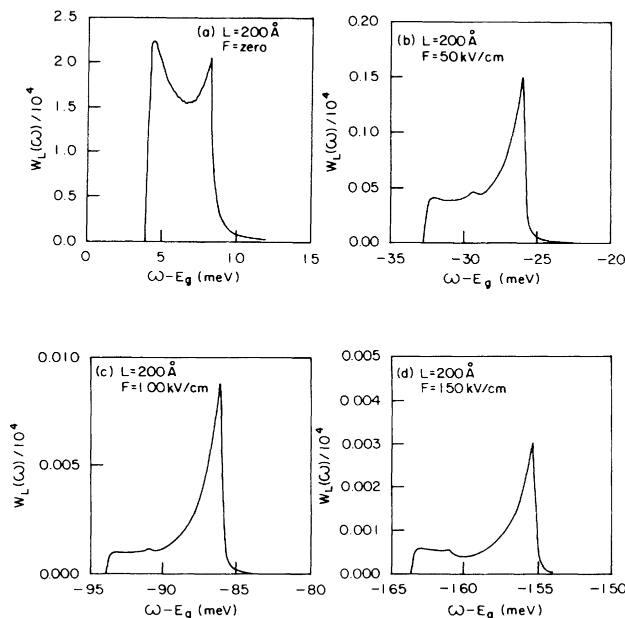

FIG. 4. Donor-related optical-absorption spectra (in units of W_0; see text) under applied electric field for a GaAs-$Ga_{0.7}Al_{0.3}As$ QW of width $L = 200$ Å. Results are presented for electric fields of (a) zero, (b) 50 kV/cm, (c) 100 kV/cm, and (d) 150 kV/cm.

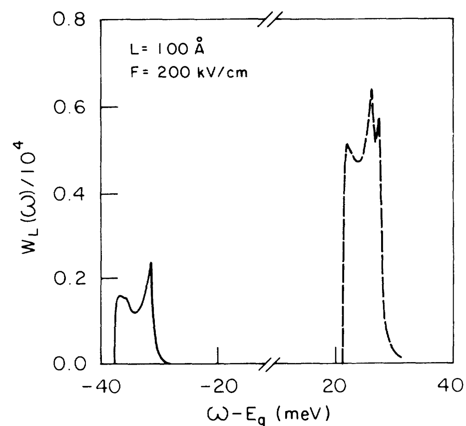

FIG. 6. Donor-related optical-absorption spectra (in units of W_0; see text) under $F = 200$ kV/cm applied electric field for a GaAs-$Ga_{0.7}Al_{0.3}As$ QW of width $L = 100$ Å. Results are presented for infinite- (dashed line) and finite- (solid curve) barrier potentials.

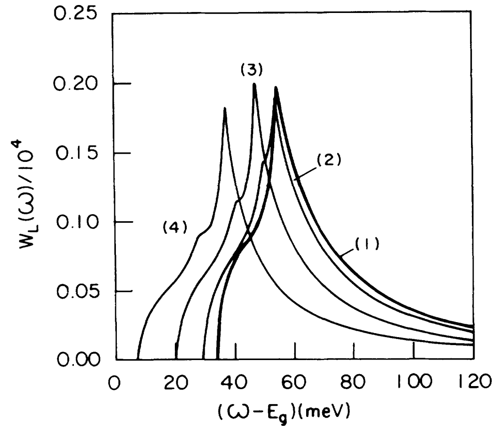

FIG. 7. Acceptor-related optical-absorption spectra (in units of W_0; see text) under applied electric field for a GaAs-$Ga_{0.7}Al_{0.3}As$ QW of width $L = 100$ Å. Results are presented for an infinite-barrier potential, and for electric fields of (1) zero, (2) 50 kV/cm, (3) 100 kV/cm, and (4) 150 kV/cm.

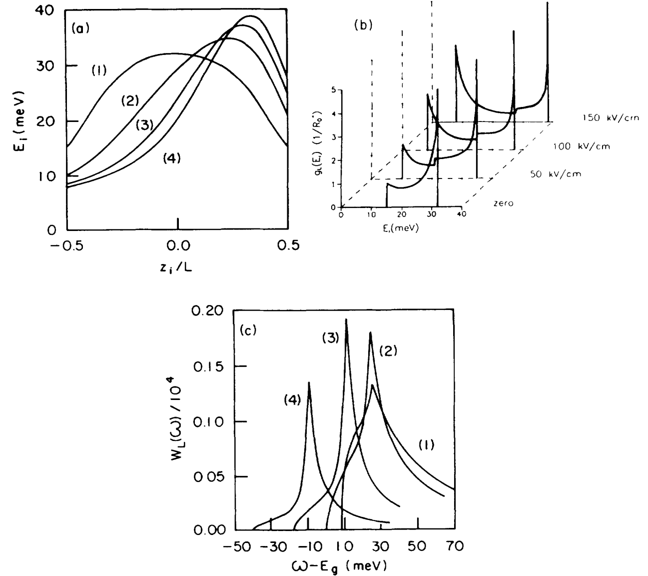

FIG. 8. (a) Impurity-position dependence of the acceptor binding energies; (b) densities of acceptor states (in reduced atomic units) as functions of the impurity binding energies $E_i = E(L, z_i)$; (c) acceptor-related optical-absorption spectra (in units of W_0; see text). Results are presented for a GaAs-$Ga_{0.7}Al_{0.3}As$ QW of thickness $L = 100$ Å and for the case of electric fields of (1) zero, (2) 50 kV/cm, (3) 100 kV/cm, and (4) 150 kV/cm.

tween the acceptor band and conduction subband and the overlap between states in these two bands. As we have previously pointed out, the overlap between states is reduced by the application of the electric field. However, the dependence of the binding-energy curve with electric field F turns out to be such that the inverse of its derivative with respect to the impurity position, i.e., the density of impurity states,[1] at $z_i = -L/2$ increases with F, whereas that at $z_i = L/2$ exhibits the opposite behavior [see Fig. 8(b)]. As a consequence, the $z_i = L/2$ van Hove–like singularity rapidly disappears with increasing F, whereas the structure associated with $z_i = -L/2$ acceptor states initially becomes more pronounced with increasing electric field (up to $F \simeq 100$ kV/cm) before having its strength reduced due to the diminishing overlap between states involved in the transition.

IV. CONCLUSIONS

We have performed a systematic analysis of the impurity-related optical-absorption line shape associated with donors and acceptors in GaAs-(Ga,Al)As QW's under the effect of an externally applied constant electric field. We have investigated the dependence of the spectra on the strength of the field and width of the QW. The absorption spectra present an edge associated to the maximum value of the impurity binding energy and two van Hove–like singularities corresponding to impurities positioned at the two edges of the QW. The latter two singularities merge into a single one in the limit of vanishing applied electric field. As the field intensity is increased, the absorption spectra are shifted towards lower energies, with their intensities reduced, and the relative importance of the van Hove–like singularities is changed. Such effects become more pronounced for increasing widths of the QW's.

To our knowledge, there are no experimental reports on the electric-field effects on the impurity-related optical-absorption line shapes in GaAs-(Ga,Al)As QW's. However, those measurements may be readily performed, and we believe the results in the present work will be relevant to the interpretation of the experimental data and understanding of the phenomena.

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