Shallow donor impurities in $GaAs/Al_xGa_{1-x}As$ superlattices in a magnetic field

J.M. Shi, F.M. Peeters, and J.T. Devreese*
Departement Natuurkunde, Universiteit Antwerpen (UIA), Universiteitsplein 1, B-2610 Antwerpen, Belgium
(Received 22 October 1993; revised manuscript received 21 March 1994)

A theoretical investigation is presented of the properties of shallow donor impurities in a $GaAs/Al_xGa_{1-x}As$ superlattice in the presence of a magnetic field directed along the growth axis. The energy levels of several of the lowest donor states have been obtained as functions of (1) the well width, (2) the donor position, and (3) the magnetic-field strength. The calculation is based on a variational approach in which we use a trial wave function with two variational parameters. This wave function shows exponential behavior in sufficiently small magnetic fields and Gaussian behavior in sufficiently large magnetic fields. The magnetopolaron effect on these donor energies is studied within second-order perturbation theory where a formal summation over *all* electron states is performed. The effect of band nonparabolicity is also included in order to correctly explain magneto-optical experimental results at high magnetic fields. Our results are in very good agreement with the available experimental data in the whole magnetic-field range and for weakly and strongly coupled superlattices.

I. INTRODUCTION

The problem of shallow donor impurities confined to a quasi-two-dimensional (Q2D) system[1] has been studied extensively during the last decade. This has become possible after the advent of material growth techniques with dimensional control close to interatomic spacing, such as molecular-beam epitaxy and metal-organic chemical-vapor deposition. The transition energies of the donor states in the low-dimensional systems have been experimentally observed by far-infrared and intersubband spectroscopy, [2–9] and various theoretical investigations[10–20] have been performed in order to understand the nature and properties of these impurities. Since the optical and transport properties of semiconductor materials are strongly influenced by both these dopant impurities and the structures of the Q2D systems, the knowledge of the effect of the confining potential barriers on the donor states is important.[21,22] Among the most extensively studied Q2D systems is the one consisting of alternating layers of GaAs and $Al_xGa_{1-x}As$.

Most of the theoretical calculations of the donor states[10–16] address the *single*-quantum well (QW) problem, which has been shown to be a good approximation for the case of an impurity located near the well center of a very weakly coupled superlattice, i.e., wide and/or high barriers and/or wide wells.[5,23] Chaudhuri[17] extended the variational calculation in a QW to a three-well structure. This work was generalized by Lane and Greene[18] to a superlattice but with a uniform electron band mass. Helm *et al.*[5] extended these calculations to all states with the principal quantum number $n \leq 2$, where they included the spatial dependence of the electron mass. These three studies were performed in the absence of any applied field. Recently, we have generalized them to include a magnetic field which is perpendicular to the $GaAs/Al_xGa_{1-x}As$ interfaces.[19]

Since polaron effects are present in polar semiconductors like GaAs, it will have influence on the position of the electronic energy levels. In particular, near the resonant magneto-polaron magnetic field the electron energies are modified appreciably. This effect on a free electron moving in a Q2D system has been studied extensively.[24–29] The case of electrons bound to donors was investigated by several groups for the QW case[14–16] and for the superlattice case.[19] In Ref. 19 we have included the polaron effect and band nonparabolicity in the calculation of the $1s \rightarrow 2p^{\pm}$ transition energies of a donor located at an arbitrary position in the superlattice. The agreement with the experimental results was reasonably good. Nevertheless, there is still room for improvement, of which the two major ones are (1) a Gaussian trial wave function was used, which is not very accurate for the donor energies in low magnetic fields.[5,30,31] Here a trial wave function will be used, which was introduced in Ref. 32 for bulk magnetodonors, which allows for an exponential behavior in the small magnetic-field limit; and (2) only three donor states $(1s, 2p^{\pm})$ were included as intermediate states in the calculation of the polaron correction. Recently,[9] we found that such a calculation underestimates the polaron correction appreciably. In the present work, we will improve on this limitation by using a formal summation over all intermediate electron states. Furthermore, we extend our previous calculation[19] to higher excited states and explain experimental data on a strongly coupled superlattice which shows a three-level resonance,[9] and on a wide-well superlattice which shows a four-level resonance.[8]

In this paper, we report on a calculation of the energy levels of the donor states $(1s,\ 2p^{\pm},\ 2p_z,\ 3d^{\pm 2},\ 4f^{\pm 3})$ for an impurity associated with the lowest two subbands of a $GaAs/Al_xGa_{1-x}As$ superlattice in an applied magnetic field which is parallel to the growth axis. The position of the donor in the superlattice is allowed to be arbi-

trary. We have included the mass discontinuity of the electron at the interface and the finite height of the barriers. To obtain the wave functions and the energy levels of the donor electron in the absence of electron-phonon interaction, a variational approach is used in which the trial wave function has two variational parameters. This function reduces to an exponential at sufficiently low magnetic fields and to a Gaussian at sufficiently high-magnetic fields. The effect of band nonparabolicity is also included. Polaron correction to these energies is calculated within second-order perturbation theory. We have been able to find an upper bound to polaron shifts for the transition energies in the nonresonant magnetic-field region by formally including *all* donor states. For the $1s \rightarrow 2p^+$ transition in the resonant magnetic-field region, we use an improved expression for the polaron correction which was recently proposed by us[31] for the three-dimensional (3D) donor. This expression is able to give the correct resonant position in high-magnetic fields, and the correct polaron shift at zero-magnetic field, although only a few relevant lowest states are effectively taken into account. A detailed comparison of the present polaron correction with the corresponding results obtained by using the more accurate treatment of Refs. 33 and 34 shows negligible differences which proves the accuracy of our approach. We find that both the polaron correction and band nonparabolicity are important in order to correctly explain the magnetopolaron resonant experimental results. Our calculation shows that the highest branch of the experimental results of Ref. 8 for the $1s \rightarrow 2p^+$ transition should be described as due to the lifting of the degeneracies between the $2p^+$ state and the ($3d^{-2}$, + one-phonon) state, which is consistent with the case of bulk GaAs.[35] In Ref. 8 these experimental data were interpreted as due to a resonant interaction between the $2p^+$ state and the ($2p_z$, + one-phonon) state.

This paper is organized as follows. In Sec. II a variational calculation of the $1s$, $2p^{\pm}$, $2p_z$, $3d^{\pm 2}$, $4f^{\pm 3}$ states of the donor in a superlattice in a magnetic field is presented in the absence of the electron-phonon interaction. The polaron correction to the energy levels of the donor is calculated in Sec. III. An improved expression for this polaron correction within second-order perturbation theory is presented. A comparison with the experimental data is given in Sec. IV. Our discussions and conclusions are presented in Sec. V.

II. VARIATIONAL CALCULATION

Within the framework of an effective-mass approximation and neglecting electronic spin, the total Hamiltonian for a single conduction-band electron in a superlattice coupled to a Coulombic impurity and interacting with longitudinal-optical (LO) phonons is given by

$$H = H_e + H_{\rm LO} + H_I, \tag{1}$$

where H_e is the electronic part

$$H_e = \left(\vec{p} + \frac{e}{c}\vec{A}\right) \frac{1}{2m_e^*(z)} \left(\vec{p} + \frac{e}{c}\vec{A}\right) - \frac{e^2}{\epsilon_0 r} + V(z), \tag{2}$$

which describes a hydrogenlike atom placed in a superlattice in an external magnetic field, where the vector potential $\vec{A}$ is chosen in the symmetric gauge, i.e., $\vec{A} = \frac{1}{2}B(-y, x, 0)$, and a uniform and constant magnetic field $\vec{B} = (0, 0, B)$ is applied along the growth axis which is taken to be the z axis of the system, c is the velocity of light in vacuum, and $-e$ the electronic charge. The potential of the superlattice is modeled by a periodic square-well potential

$$V(z) = \begin{cases} 0, & -w/2 + nl < z < w/2 + nl \\ V_0, & w/2 + nl < z < w/2 + b + nl, \end{cases} \tag{3}$$

with w the well width, b the barrier width, $l = w + b$ the periodicity, and $n = 0, \pm 1, \pm 2, \cdots$, an integer. For the GaAs/$Al_xGa_{1-x}As$ interfaces the barrier height V_0 depends on the Al concentration x in the barriers, and is given by 60% of the total energy-band-gap difference between GaAs and $Al_xGa_{1-x}As$: $\Delta E_g = 1.155x + 0.37x^2$ eV.[36] The position of the donor electron is denoted by $\vec{r}$, $r = \sqrt{\rho^2 + (z - z_I)^2}$ is the distance between the electron and the donor center with $\rho = \sqrt{x^2 + y^2}$ being the distance in the xy plane, and $(0, 0, z_I)$ is the position of the donor center. The quantity $m_e^*(z)$ is the electron effective mass, which is different in the two semiconductors: for the GaAs wells $m_w/m_e = 0.067$ (m_e the electronic mass in vacuum), and for the $Al_xGa_{1-x}As$ barriers $m_b/m_e = 0.067 + 0.083x$. $\epsilon_0 = 12.75$ is the static dielectric constant of GaAs,[35] which is taken to be the same in both materials which is a good approximation for the GaAs/$Al_xGa_{1-x}As$ superlattice.

In Eq. (1), $H_{\rm LO}$ is the LO-phonon Hamiltonian which is given by

$$H_{\rm LO} = \sum_{\vec{q}} \hbar\omega_{\vec{q}} \left(a_{\vec{q}}^{\dagger} a_{\vec{q}} + \frac{1}{2}\right), \tag{4}$$

where $a_{\vec{q}}^{\dagger}$ ($a_{\vec{q}}$) is the creation (annihilation) operator of a LO phonon with momentum $\hbar\vec{q}$ and energy $\hbar\omega_{\vec{q}}$. For GaAs we take $\hbar\omega_{\vec{q}} = \hbar\omega_{\rm LO} = 36.75$ meV independent of the phonon momentum at $T = 4.2$ K which is the considered experimental region.[37]

The electron-phonon interaction in Eq. (1) is given by

$$H_I = \sum_{\vec{q}} (V_{\vec{q}}\, a_{\vec{q}}\, e^{i\vec{q}\cdot\vec{r}} + V_{\vec{q}}^*\, a_{\vec{q}}^{\dagger} e^{-i\vec{q}\cdot\vec{r}}), \tag{5}$$

where

$$|V_{\vec{q}}|^2 = \frac{4\pi\alpha}{\Omega} \sqrt{\frac{\hbar}{2m_w\omega_{\rm LO}}} \left(\frac{\hbar\omega_{\rm LO}}{q}\right)^2$$

with Ω the system volume, and

$$\alpha = \frac{e^2}{\hbar} \sqrt{\frac{m_w}{2\hbar\omega_{\rm LO}}} \left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)$$

the standard Fröhlich coupling constant, and ϵ_∞ the high frequency dielectric constant of GaAs. In our calculation we take $\alpha = 0.068$,[37] being the value for GaAs. Furthermore, we take only the interaction with 3D-bulk GaAs phonon modes and in so doing we neglect the effect of

the structure of the superlattice on the phonon modes.

Because the magnetic field is applied along the growth axis, it is convenient to discuss our problem using cylindrical polar coordinates (ρ, ϕ, z) in which the electronic Hamiltonian H_e can be reduced to the following form:

$$H_e = -\frac{m_w}{m_e^*(z)}\left(\nabla^2 + i\gamma\frac{\partial}{\partial\phi} - \frac{1}{4}\gamma^2\rho^2\right) - \frac{2}{r} + V(z), \quad (6)$$

where the effective Bohr radius in GaAs, $a_0^* = \hbar^2\epsilon_0/m_w e^2 = 100.7$ Å, is taken as the unit of length, the effective Rydberg $\mathcal{R}^* = e^2/2\epsilon_0 a_0^* = 5.61$ meV as the unit of energy, and γ is a dimensionless measure of the magnetic field, $\gamma = e\hbar B/2m_w c\mathcal{R}^* = 0.154B$ (T). Notice that the magnetic quantum number m of the donor state, which is connected to $L_z = -i\hbar(\partial/\partial\phi)$, the z component of the angular momentum operator, commutes with the total Hamiltonian. Thus m is still a good quantum number for all magnetic-field strengths. For the states of the donor located at the well or barrier center the z-parity quantum number p is also a good quantum number. But the other 3D equivalent quantities such as the principal quantum number and the angular quantum number are no longer good quantum numbers.

The Schrödinger equation with the Hamiltonian H_e cannot be solved exactly. A variational calculation for the $1s$, $2p^{\pm}$, $2p_z$, $3d^{\pm 2}$, and $4f^{\pm 3}$ states of the donor will be given. Since in general the electron energy related to the superlattice potential is much larger than the Coulomb energy, one can explicitly factor out the associated subband solution of the one-dimensional superlattice potential from the wave function of the donor. Therefore, the variational wave function of the donor state can be written as the product of two functions

$$\Psi(\rho, \phi, z) = f_{j,k_z}(z)\psi(\rho, \phi, z - z_I), \quad (7)$$

where $f_{j,k_z}(z)$ is the lowest-energy-edge solution of the jth subband of the one-dimensional superlattice, which has momentum $\hbar k_z$ and energy E_{j,k_z}, and is periodically repeated in the z direction, i.e., $f_{j,k_z}(z) = e^{ik_z nl} f_{j,k_z}(z + nl)$ with n an integer. The $j = 1, 3, 5, \ldots$ subbands of the superlattice are built from the hybridization of the isolated well eigenstates which are even, while the $j = 2, 4, 6, \ldots$ subbands arise from hybridizing the odd eigenstates of the isolated wells. The lowest-energy edges of the subbands are given by $k_z = 0$ for $j =$ odd and by $k_z = \pi/l$ for $j =$ even. Thus, for the lower edges of the odd-number subbands one can write

$$f_{j,0}(z) = \begin{cases} \cos(k_w z), & |z| < w/2 \\ B_1 \cosh(k_b z), & w/2 < z < w/2 + b, \end{cases} \quad (8a)$$

with the energy $E_{j,0}$ given by

$$\cos\left(\frac{k_w w}{2}\right)\sinh\left(\frac{k_b b}{2}\right) - \frac{k_w m_b}{k_b m_w}\sin\left(\frac{k_w w}{2}\right)\cosh\left(\frac{k_b b}{2}\right) = 0, \quad (8b)$$

while for the even-number subbands one has

$$f_{j,\pi/l}(z) = \begin{cases} \sin(k_w z), & |z| < w/2 \\ B_2 \cosh(k_b z), & w/2 < z < w/2 + b, \end{cases} \quad (8c)$$

with the energy $E_{j,\pi/l}$ given by

$$\sin\left(\frac{k_w w}{2}\right)\sinh\left(\frac{k_b b}{2}\right) + \frac{k_w m_b}{k_b m_w}\cos\left(\frac{k_w w}{2}\right)\cosh\left(\frac{k_b b}{2}\right) = 0. \quad (8d)$$

The coefficients k_w, k_b, B_1, B_2 of the wave functions $f_{j,k_z}(z)$ are determined by the current-conserving boundary conditions at the interfaces, which implies that both $f_{j,k_z}(z)$ and $[1/m_e^*(z)][\partial f_{j,k_z}(z)/\partial z]$ are continuous across the interfaces[38] which results in

$$k_w = \sqrt{E_{j,k_z}}, \qquad k_b = \sqrt{\frac{m_b}{m_w}(V_0 - E_{j,k_z})},$$

and

$$B_1 = \frac{\cos(k_w w/2)}{\cosh(k_b w/2)}, \qquad B_2 = \frac{\sin(k_w w/2)}{\cosh(k_b w/2)}.$$

The wave functions which correspond to the edge solutions of the two lowest subbands of a $GaAs/Al_{0.3}Ga_{0.7}As$ superlattice are shown in Fig. 1 for $w = 75$ Å and $b = 25$ Å. We notice that (1) the first subband has even z parity, and has no node for the lower edge ($k_z = 0$, solid curve) and one node for the upper edge ($k_z = \pi/l$, dashed curve), while the second subband has odd z parity, and has one node for the lower edge ($k_z = \pi/l$, dotted curve) and two nodes for the upper edge ($k_z = 0$, dash-dotted curve); (2) the electronic states in the first subband have

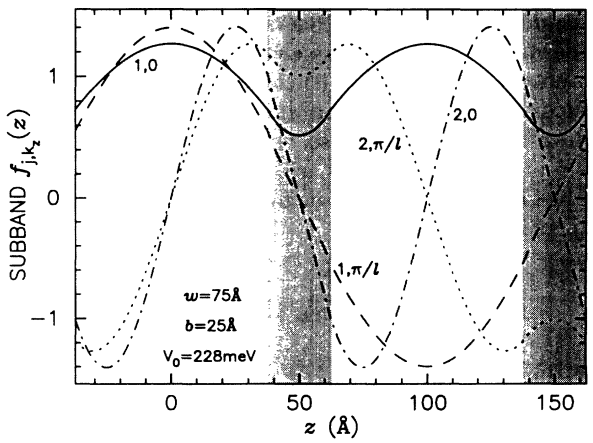

FIG. 1. The subband wave functions corresponding to the energy miniband edges of the two lowest subbands of a $GaAs/Al_{0.3}Ga_{0.7}As$ superlattice with well width $w = 75$ Å and barrier width $b = 25$ Å. The position of the latter is indicated by the shaded area. The lower and the upper edges of the first subband are given by solid and dashed curves, and those of the second subband by dotted and dash-dotted curves, respectively.

their maximum probability density at the well center, while those in the second subband have it near the barriers; (3) the even z-parity states of the donor under study ($1s$, $2p^{\pm}$, $3d^{\pm 2}$, $4f^{\pm 3}$) should be associated with the lower edge $[f_{1,0}(z)]$ of the first subband, and the odd z-parity $2p_z$ state with the lower edge $[f_{2,\pi/l}(z)]$ of the second subband; and (4) the presence of the barriers lifts the degeneracy between the $2p^{\pm}$ and $2p_z$ states at $B = 0$. The magnetic field will further lift the degeneracy between the $2p^{+}$ and $2p^{-}$ states.

The second part $\psi(\rho, \phi, z - z_I)$ of the wave function Ψ describes the localized part. For the wave function of the donor in a superlattice we take the following form:

$$\Psi_{j,m,p}(\rho, \phi, z - z_I) = f_{j,p\pi/l}(z)\rho^{|m|}e^{im\phi}e^{-\eta\rho^2 - \xi\sqrt{\rho^2 + (z-z_I)^2}}, \quad (9)$$

where η and ξ are two variational parameters. Apart from the superlattice miniband wave function $f_{j,k_z}(z)$ the above form is similar to the one proposed in Ref. 32 for 3D magneto-donor states. The different states are indicated by the three quantum numbers (j, m, p) as follows: $1s(1,0,0)$, $2p^{\pm}(1,\pm 1,0)$, $2p_z(2,0,1)$, $3d^{\pm 2}(1,\pm 2,0)$, and $4f^{\pm 3}(1,\pm 3,0)$. The above mentioned states are orthogonal to each other by construction and have the same symmetry (for $z_I = 0$) as the corresponding 3D hydrogenic states. For low magnetic fields these functions reduce to exponential (i.e., $\eta < \xi$) and to Gaussian at sufficiently high-magnetic fields (i.e., $\eta > \xi$). The two variational parameters (η, ξ) for each state, e.g., the (j, m, p) state, are determined such that they minimize the unperturbed energy of this state

$$E^0_{j,m,p} = \frac{\langle \Psi_{j,m,p}|H_e|\Psi_{j,m,p}\rangle}{\langle \Psi_{j,m,p}|\Psi_{j,m,p}\rangle}. \quad (10)$$

In the variational calculation one only needs the states with $m \geq 0$ since

$$E^0_{j,-|m|,p} = E^0_{j,|m|,p} - 2|m|\gamma A(\Psi_{j,m,p}), \quad (11)$$

which is different from that in a 3D system where the effective mass of the electron is constant (i.e., $A = 1$). The factor, $A(\Psi) = \langle \Psi|m_w/m^*_e(z)|\Psi\rangle/\langle \Psi|\Psi\rangle$, appears in Eq. (11) since the effective mass of the electron is different in the well material, GaAs, and in the barrier material, $Al_xGa_{1-x}As$. This results in the fact that the energy difference between the $2p^{+}$ and $2p^{-}$ states is no longer equal to $\hbar\omega_c$ (i.e., 2γ), where $\omega_c = eB/m_wc$ is the cyclotron resonant frequence for a noninteracting electron in GaAs.

We also tried to improve our theoretical results by including the subband structure of the superlattice into the donor wave function (9). Explicitly, $f_{j,p\pi/l}(z)$ was replaced by a linear combination of $f_{j,k_z}(z)$. We found that this did not lead to any significant improvements in the donor energy for the superlattices studied in the present work. For the $1s \rightarrow 2p^{+}$ transition energy differences were found which are less than $0.03\mathcal{R}^*$ in the magnetic-field region $0 \rightarrow 25$ T.

III. POLARON CORRECTION

The GaAs/$Al_xGa_{1-x}As$ superlattices under investigation are weakly polar material and as a consequence the energy levels of the electron are influenced by the polarization of the medium around the electron. This is described as a polaron correction to the energy of the ith $[i = (j, m, p)]$ state of the donor which we calculate within second-order perturbation theory

$$\Delta E_i = -\sum_{i'}\sum_{\vec{q}} \frac{|\langle \Psi_{i'}; \vec{q}|H_I|\Psi_i; \vec{0}\rangle|^2}{\hbar\omega_{\vec{q}} + E^0_{i'} - E^0_i - \Delta_i}, \quad (12)$$

where $\Delta_i = 0$ for all states in the polaron nonresonant region which corresponds to Rayleigh-Schrödinger perturbation theory, and $\Delta_{2p^+} = \Delta E_{2p^+} - \Delta E_{1s}$ for the $2p^{+}$ state which corresponds to the improved Wigner-Brillouin-perturbation theory.[26,39] $|\Psi_i; \vec{q}\rangle$ describes a state composed of a donor electron with unperturbed energy E^0_i and a LO phonon with momentum $\hbar\vec{q} = \hbar(\vec{q}_{\parallel}, q_z)$ and energy $\hbar\omega_{\vec{q}}$.

In Fig. 2 the numerical results for the eighteen matrix elements of $H_I^{i,i'} = \sum_{\vec{q}}|\langle \Psi_{i'}; \vec{q}|H_I|\Psi_i; \vec{0}\rangle|^2$, in units of $(\mathcal{R}^*)^2$, for a donor located at the well center ($z_I = 0$ Å, solid curves) of the superlattice with $x = 0.25$ and $w = b = 100$ Å are presented as a function of the magnetic field. The corresponding results of the diagonal matrix elements for the barrier-center donor ($z_I = 100$ Å) are also plotted and shown by dotted curves in the left figure for comparison. Notice that (1) all the values of these matrix elements increase with increasing magnetic field, which is due to the fact that increasing the magnetic field will bind the electron nearer to the donor center and increase the overlap of the wave functions; (2) the diagonal $H_I^{i,i}$ matrix elements [Fig. 2(a)] are larger than the others [Figs. 2(b) and 2(c)], and the less localized states have smaller values; (3) the value of the matrix element $H_I^{i,i'}$ is smaller when the two states (i, i') have a large difference in magnetic moment and/or energy; (4) there are some crossings of the curves, which are a consequence of the different dependence of the width of the state on the magnetic field. For instance, the crossing of the $H_I^{2p^{\pm},2p^{\pm}}$ and $H_I^{2p_z,2p_z}$ matrix elements at $\gamma \sim 1.6$ is due to the fact that the width of the $2p^{\pm}$ state with larger magnetic moment decreases with increasing magnetic field more rapidly than that of the $2p_z$ state which has zero-magnetic moment; (5) the effect of the electron-phonon interaction on the well-center donor is stronger than on the barrier-center donor as the width of the donor states is an increasing function of the donor distance from the well center (see Fig. 3 of Ref. 19); and (6) the polaron effect on donor states in a Q2D system is stronger than in bulk material (see Fig. 4 of Ref. 31) due to the confinement from the barriers.

It is possible to evaluate Eq. (12) approximately and to perform the sum $\sum_{i'}$ formally such that one needs to know only a few relevant states in order to calculate the polaron shift to the energy levels of the well- and barrier-center donors.[40,41] Using the method, which is described

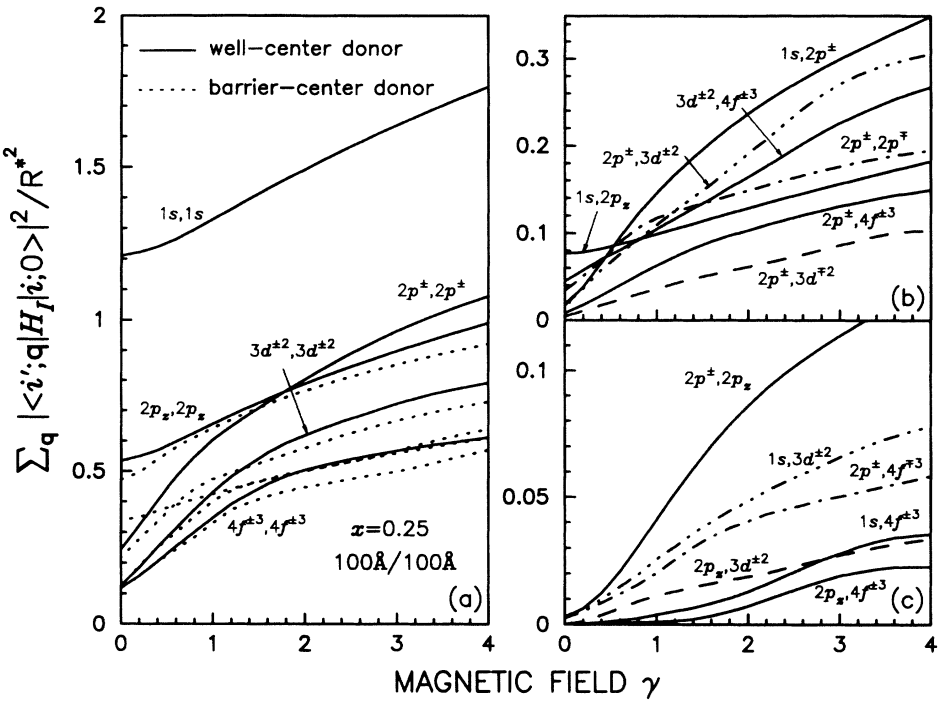

FIG. 2. The values of the electron-phonon transition matrix elements, $H_I^{i,i'}$, in units of $(\mathcal{R}^*)^2$, are plotted as a function of the magnetic field γ for the well-center donor (solid curves) in a superlattice with $x = 0.25$ and $w = b = 100$ Å. As a comparison those of the diagonal matrix elements for the barrier-center donor are also given by the dotted curves in the left figure.

in detail in Ref. 31, with the approximation $m_w = m_b$ we found the following approximations to Eq. (12). The first one is

$$\Delta E_i = -\alpha\hbar\omega_{\rm LO} - \frac{2\alpha}{3}\frac{\langle\Psi_i|(\vec{p}+\frac{e}{c}\vec{A})^2|\Psi_i\rangle}{\langle\Psi_i|\Psi_i\rangle}, \qquad (13)$$

which is only valid for (i) the nonresonant states, and (ii) the states such that $E^0_{i'} - E^0_i \ll \hbar\omega_{\rm LO}$ in low-magnetic fields, and $E^0_{i'} - E^0_i \ll \hbar\omega_{\rm LO}$ or $E^0_{i'} - E^0_i > 0$ in high-magnetic fields, for which we take $\Delta_i = 0$. In the case of the ground state we can prove that Eq. (13) is an upper bound to the polaron correction (12). For the $2p^+$ state we follow Ref. 31 and find

$$\Delta E_{2p^+} = \Delta E_{2p^-} - \sum_{i=2p^\pm}\sum_{i'}\sum_{\vec{q}}\frac{m_i|\langle\Psi_{i'};\vec{q}|H_I|\Psi_i;\vec{0}\rangle|^2(E^0_{i'} - E^0_i - q^2)^2}{(\hbar\omega_{\rm LO} + E^0_{i'} - E^0_i - \Delta_i)(\hbar\omega_{\rm LO} + q^2)^2}. \qquad (14)$$

This expression has the following desirable properties: (1) at $\gamma = 0$ the polaron correction to the $2p^+$ state is identical to the one of the $2p^-$ state, which is due to the fact that in this limit both states are identical; (2) for $\gamma > 0$ $|\Delta E_{2p^+}|$ is larger than $|\Delta E_{2p^-}|$ since the former is related to the second ($N = 1$) Landau level of the free electron, and the latter to the lowest ($N = 0$) Landau level; and (3) at resonance it is able to give the correct resonant position since we have included the relevant resonant states in the sum $\sum_{i'}$.

We have examined the accuracy of the above expressions Eqs. (13) and (14) by comparing their numerical results with those obtained from the method used by Cohn, Larsen, and Lax[33] for the polaron corrections to the $1s \to 2p^\pm$ transition energies as a function of the magnetic fields up to 25 T in the 80 Å/9 Å superlattice. A comparison was also made between the method of Ref. 33 and the one used in Ref. 19. We found that for the $1s \to 2p^\pm$ transition energies the differences are less than 2 $\rm cm^{-1}$ and 4 $\rm cm^{-1}$ for the present approach and the one of Ref. 19, respectively.

We depict in Fig. 3 the unperturbed energy levels of the $1s$, $2p^\pm$, $2p_z$, $3d^{-2}$, and $4f^{-3}$ states (dotted curves) together with the same ones shifted over a LO-phonon energy (dash-dotted curves), and the energy levels including the polaron correction (solid curves) for a well-center donor in a superlattice with $x = 0.23$, $w = 450$ Å, and $b = 125$ Å, where the polaron correction is calculated by using Eq. (14) for the $2p^+$ state, and Eq. (13) for the others. Notice that (1) for not too large magnetic fields the polaron correction shifts the energy levels to lower energy, and these shifts increase with increasing magnetic-field strength; and (2) at resonance (i.e., $E^0_{2p^+} = E^0_i + \hbar\omega_{\rm LO}$ for $i \neq 2p^+$), there is a crossing of the unperturbed levels. The electron-phonon interaction lifts this degeneracy, and leads to a splitting of these energy levels; (3) the rapid increase of the polaron correction to the $2p^+$ state (see the lowest branch) for $\gamma > 1.5$ is a result of the fact that this state is moving close to resonance; (4) since the $2p_z$ state is higher ($\sim 1\mathcal{R}^*$) in energy

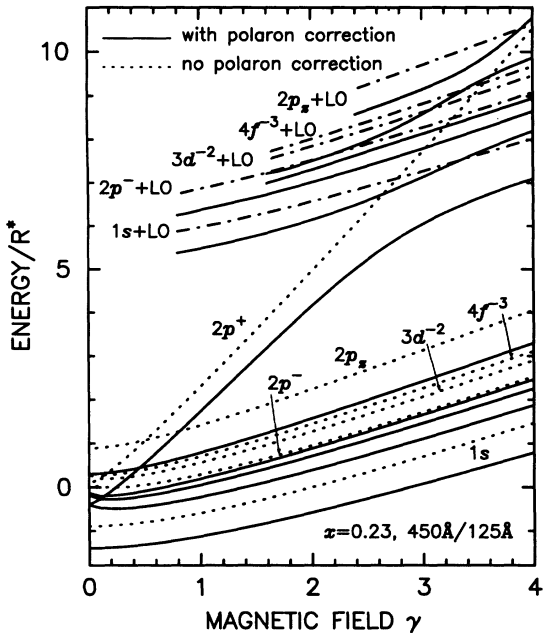

FIG. 3. Energy levels of a donor at the well center of the superlattice with $x = 0.23$, $w = 450$ Å, and $b = 125$ Å as a function of the magnetic field with (solid curves) and without (dotted curves) the electron-phonon interaction. The dash-dotted curves are the energy levels of the unperturbed states shifted by a LO phonon.

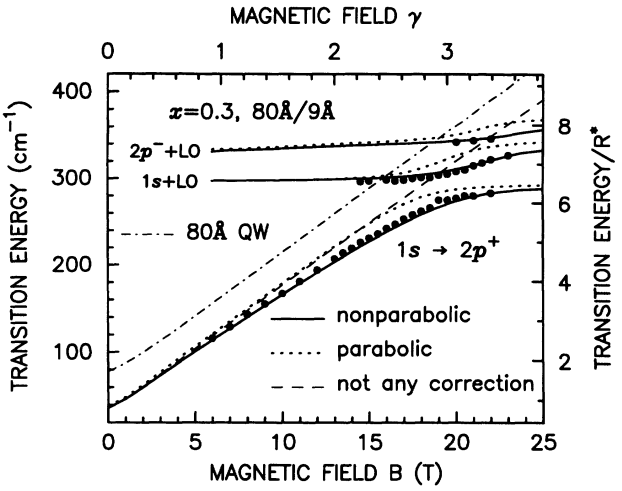

FIG. 4. The $1s \rightarrow 2p^+$ transition energy as a function of the magnetic field for a well-center donor in a strongly-coupled $GaAs/Al_{0.3}Ga_{0.7}As$ superlattice with $w = 80$ Å and $b = 9$ Å. We show our theoretical results for the following cases: (a) without the polaron effect for a parabolic band (dashed curve); (b) with the polaron correction (dotted curves); and (c) including the effects of polaron and band nonparabolicity (solid curves). The dash-dotted curve indicates the result for the QW case without any correction. The experimental data (solid dots) are from Ref. 9.

than those of the other states, with the exception of the $2p^+$ state, we do not expect it to be so important as the others in the process of the resonant polaron splitting. This is consistent with the 3D case,[31] and is important in the interpretation of the experimental results of Cheng *et al.*[8] In fact, the energy levels of the donor in this superlattice should be similar to those in bulk GaAs because of its very wide wells.

IV. COMPARISON WITH EXPERIMENTS

In this section we will compare our theoretical results to available experimental data. In Ref. 19 many experimental results have been very well described, although (1) the Gaussian wave function was invoked for the variational calculation, and (2) only three donor states $(1s, 2p^{\pm})$ were included in the polaron correction. The reason is that all the experiments mentioned there were done in the weakly-coupled superlattices, and the results were only for the low-energy transitions, and/or two- and three-level resonances.

First, we consider the donor in a strongly-coupled superlattice. Recently, the $1s \rightarrow 2p^+$ transition energies of the donor located at the well center of a superlattice with $x = 0.3$, $w = 80$ Å, and $b = 9$ Å were observed.[9] A three-level resonance was found. These results are plotted in Fig. 4 as function of the magnetic field, and shown as the solid dots. The calculated results (dashed curve) without polaron correction can not explain the higher branches of the $1s \rightarrow 2p^+$ transition, although they are in reasonable good agreement with the experimental results in low-magnetic fields. As a reference the theoretical results for the case of a QW with well width $w = 80$ Å are also indicated by the dash-dotted curve, which overestimates greatly the transition energy. Therefore, the theory of a *single*-quantum well does not work at all here. The present results including polaron correction are given by the dotted curves. Notice that (1) the polaron effect in lower magnetic fields ($B < 15$ T) is very small, and shifts the transition energy to higher levels. In this region the polaron correction to the ground state is larger than to the $2p^+$ state; (2) at resonance a three-level resonance is found, which is due to the energy splitting of the $2p^+$ state and the $|\Psi_{1s}; \vec{q}\rangle$ and $|\Psi_{2p^-}; \vec{q}\rangle$ states; and (3) the agreement between theory and experiment is only good in the low-magnetic-field region. It becomes unsatisfactory for all the three branches at higher magnetic fields, where the effect of band nonparabolicity on the energy of the donor electron becomes important.

Band nonparabolicity is included using the standard Kane model

$$E_{\rm np} = \frac{E_g}{2}\left(-1 + \sqrt{1 + \frac{4E_p}{E_g}}\right), \tag{15}$$

where E_{np} and E_p are the donor energies with and without the effect of band nonparabolicity, respectively, $E_g = 1.52$ eV is the band gap of GaAs. This expression has been used successfully to describe band nonparabolicity both for free electron cyclotron resonance in GaAs heterostructures[42] and for the donor transition energy

in bulk GaAs.[35] The results for the $1s \rightarrow 2p^+$ transition energies including the polaron correction and band nonparabolicity are given by the solid curves in Fig. 4. Now our theoretical results are in very good agreement with the experimental data. It is apparent that the effect of band nonparabolicity decreases the transition energies because it diminishes the energy of the excited state more than that of the ground state. Although there is good agreement, we notice that at resonance ($B = 20$ T) the experimental splitting, i.e., the difference between the lowest two branches, $\Delta = 21$ cm^{-1} is slightly (16%) smaller our theoretical result $\Delta = 25$ cm^{-1}. It is not clear if this is due to an experimental inaccuracy or an inaccuracy in our theoretical model.

Huant and co-workers[3,6] have measured the $1s \rightarrow 2p^+$ transition energies of donors located at the well center and the barrier center of a superlattice with $x = 0.25$ and $w = b = 100$ Å which is a weakly-coupled superlattice. A two-level resonance for the well-center donor was found, which is due to a resonant interaction between $2p^+$ and the $|\Psi_{1s};\vec{q}\rangle$. We compare these measured results (solid dots) to our theoretical results in Fig. 5. It is found that our calculation (solid curves) can describe very well these experimental data if the effects of polaron and band nonparabolicity are included. However, we would like to mention that from Fig. 9 of Ref. 19 one can see that the Gaussian wave function is already a good approximation to describe the donor states in this system, although here we found a little improvement of the theory which is under 1%.

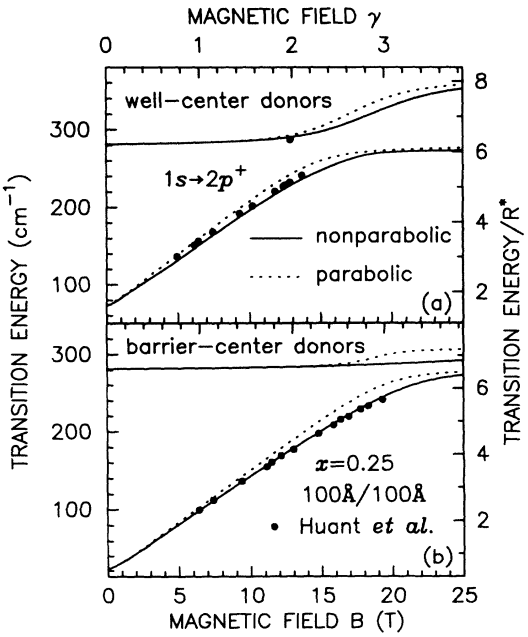

FIG. 5. Energies of the $1s \rightarrow 2p^+$ transition vs the magnetic field for a donor located at (a) the well center, and (b) at the barrier center of an $x = 0.25$, $w = b = 100$ Å superlattice. We show our calculated results including polaron correction for the cases including band nonparabolicity (solid curves) and for a parabolic band (dotted curves). The experimental data (solid dots) are from Huant and co-workers (Refs. 3 and 6).

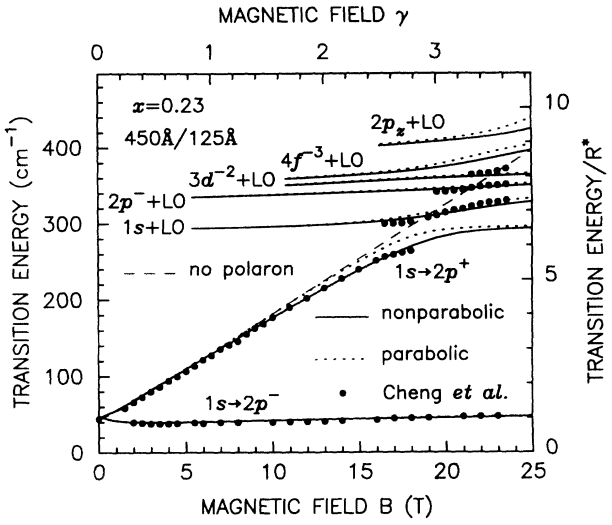

FIG. 6. The $1s \rightarrow 2p^{\pm}$ transition energies as a function of the magnetic field for a donor at the well center of the superlattice with $x = 0.23$, $w = 450$ Å, and $b = 125$ Å. The results are shown with (solid curves) and without (dotted curves) band nonparabolicity, and compared to the experimental data (solid dots) from Ref. 8.

Recently Cheng *et al.* were able to observe a four-level resonance of the $1s \rightarrow 2p^+$ transition of the donor at the well center of a GaAs/$Al_{0.23}Ga_{0.77}As$ superlattice with $w = 450$ Å and $b = 125$ Å,[8] and also a six-level resonance of this transition in bulk GaAs.[35] The experimental results for the 3D case have been satisfactorily explained in Ref. 35. The experimental results for the superlattice case are plotted in Fig. 6 by solid dots. A good agreement is found between theory and experiment over the whole magnetic-field range. Cheng *et al.*[8] have argued previously that the highest branch of the resonance is from the resonant LO-phonon interaction between the $2p^+$ and the $|\Psi_{2p_z};\vec{q}\rangle$ states due to that the energy level of $2p_z$ is closer to that of $2p^-$ than those of the other excited states. But we found that is not true for the present situation. Notice that (1) the "interaction energy gap" between the highest two branches of the experimental results is about $0.5\mathcal{R}^*$, while the minimum energy difference of the $2p_z$ and $2p^-$ states from our calculation is about $0.8\mathcal{R}^*$ at $\gamma = 0.0$, and (2) the energy levels of $3d^{-2}$ and $4f^{-3}$ are lower than that of $2p_z$ in the whole magnetic-field region (see Fig. 3), which indicates that these two states are more important than $2p_z$. Our calculation, as in the 3D case, shows that the highest branch of the experimental results should be attributed to the lifting of the $E^0_{2p^+}$ and $E^0_{3d^-2} + \hbar\omega_{\rm LO}$ degeneracy, instead of $E^0_{2p^+}$ and $E^0_{2p_z} + \hbar\omega_{\rm LO}$.

V. DISCUSSION AND CONCLUSION

Using a variational approach we have investigated the energy levels of shallow donor impurities in

GaAs/$Al_xGa_{1-x}As$ superlattices in the presence of a magnetic field along the growth axis. The position of the donor in the superlattice can be chosen arbitrary. The electron-LO-phonon correction to these energy levels was included within second-order perturbation theory. We find that the polaron effect decreases the energy of the donor state in low-magnetic fields, and leads to a resonant splitting of the energies at high-magnetic fields. In order to correctly describe the experimental results the effect of band nonparabolicity on the donor states must be included which turns out to be important at high-magnetic fields. Furthermore, the present study shows that (1) the single-quantum-well theory is not a good approximation for the strongly-coupled superlattice, and (2) the Gaussian wave function gives satisfactory results for the weakly-coupled superlattice with not too wide wells. Our calculation, without *any* fitting parameters, is in good agreement with the available experimental data.

In discussing the experimental data, we found that there are still two small discrepancies (see, e.g., Fig. 4): (i) below the LO-phonon energy the experimental results are just above the calculated results including the effect of band nonparabolicity, but below the results for a parabolic conduction band. This may indicate that the effect of band nonparabolicity is slightly overestimated; and (ii) the gap at the anticrossing point is theoretically slightly overestimated as compared to experiment. Nevertheless, we know that in this energy region one is in the reststrahlen band of GaAs and the radiation is strongly absorbed by the lattice. We found no direct evidence for the interaction of the electron with nonbulk LO phonons, even in the case of the strongly-coupled superlattice. This may indicate that the polaron effect due to the nonbulk LO phonons has the same magnitude and effect as the one from bulk LO phonons in the GaAs/$Al_xGa_{1-x}As$ superlattices discussed in the present work.

ACKNOWLEDGMENTS

One of us (F.M.P.) is supported by the Belgian National Science Foundation. We are grateful to B.D. McCombe and J.P. Cheng for providing us with their experimental data prior to publication. Part of this work is sponsored by "Diensten voor de Programmatie van het Wetenschapsbeleid" (Belgium) under Contract No. IT/SC/24.

* Also at RUCA, B-2020 Antwerpen, Belgium and Technical University Eindhoven, The Netherlands.

[1] A.A. Reeder, J.M. Mercy, and B.D. McCombe, IEEE J. Quantum Electron. **QE-24**, 1690 (1988), and references therein.

[2] N.C. Jarosik, B.D. McCombe, B.V. Shanabrook, J. Comas, J. Ralsto, and G. Wicks, Phys. Rev. Lett. **54**, 1283 (1985).

[3] S. Huant, W. Knap, G. Martinaz, and B. Etienne, Europhys. Lett. **7**, 159 (1988).

[4] J.P. Cheng and B.D. McCombe, Phys. Rev. B **42**, 7626 (1990).

[5] M. Helm, F.M. Peeters, F. DeRosa, E. Colas, J.P. Harbison, and L.T. Florez, Phys. Rev. B **43**, 13 983 (1991).

[6] S. Huant, S.P. Nadja, W. Knap, G. Martinez, B. Etienne, C.J.G.M. Langerak, J. Singleton, R.A.J. Thomeer, G. Hai, F.M. Peeters, and J.T. Devreese, in *Proceedings of the 20th International Conference on the Physics of Semiconductors*, edited by E.M. Anastassakis and J.D. Joannopoulos (World Scientific, Singapore, 1990), p. 1369.

[7] G. Brozak and B.D. McCombe, Phys. Rev. B **40**, 1265 (1989).

[8] J.P. Cheng, B.D. McCombe, and G. Brozak, *Proceedings of the 5th International Conference on Modulated Semiconductor Structures* (Nara, Shin-Kohkaido, Japan, 1991); J.P. Cheng, B.D. McCombe, G. Brozak, and W. Schaff, Phys. Rev. B **48**, 17 243 (1993).

[9] F.M. Peeters, J.M. Shi, J.T. Devreese, J.P. Cheng, B.D. McCombe, and W. Schaff, Solid-State Electron. **37**, 1217 (1994).

[10] G. Bastard, Phys. Rev. B **24**, 4714 (1981).

[11] C. Mailhoit, Y.C. Chang, and T.C. McGill, Phys. Rev. B **26**, 4449 (1982).

[12] R.L. Greene and K.K. Bajaj, Phys. Rev. B **31**, 913 (1985).

[13] S. Chaudhuri and K.K. Bajaj, Phys. Rev. B **29**, 1803 (1984).

[14] C.D. Hu and Y.H. Chang, Phys. Rev. B **40**, 3878 (1989).

[15] F.A.P. Osório, M.Z. Maialle, and O. Hipólito, in *Proceedings of the 20th International Conference on the Physics of Semiconductors* (Ref. 6), p. 1017.

[16] D.L. Lin, R. Chen, and T.F. George, Phys. Rev. B **43**, 9382 (1991).

[17] S. Chaudhuri, Phys. Rev. B **28**, 4480 (1983).

[18] P. Lane and R.L. Greene, Phys. Rev. B **33**, 5871 (1986).

[19] J.M. Shi, F.M. Peeters, G.Q. Hai, and J.T. Devreese, Phys. Rev. B **44**, 5692 (1991).

[20] E.P. Pearl, J.L. Dunn, and C.A. Bates, J. Phys. Condens. Matter **4**, L199 (1992).

[21] W.T. Masselink, Y.C. Chang, H. Morkoç, D.C. Reynolds, C.W. Litton, K.K. Bajaj, and P.W. Yu, Solid-State Electron. **29**, 205 (1986).

[22] B.D. McCombe, N.C. Jarosik, and J.M. Mercy, in *Two-Dimensional Systems: Physics and New Devices*, edited by G. Bauer, G. Kuchar, and H. Heinrich (Springer-Verlag, Berlin, 1986), p. 156.

[23] J.T. Devreese, J.M. Shi, and F.M. Peeters, in *Phonons in Semiconductor Nanostructures*, edited by J.P. Leburton *et al.* (Kluwer, Dordrecht, 1993), p. 173.

[24] S.D. Sarma and A. Madhukar, Phys. Rev. B **22**, 2823 (1980).

[25] R. Lassnig and W. Zawadzki, Surf. Sci. **142**, 388 (1984).

[26] F.M. Peeters and J.T. Devreese, Phys. Rev. B **31**, 3689 (1985).

[27] D.M. Larsen, Phys. Rev. B **40**, 4595 (1987).

[28] F.M. Peeters, X.G. Wu, and J.T. Devreese, Solid State Commun. **65**, 1505 (1988).

[29] M.H. Degani and O. Hipólito, Superlatt. Microstruct. **5**, 141 (1989).

[30] F.M. Peeters, J.M. Shi, and J.T. Devreese, in *Optical Phe-*

nomena in Semiconductor Structures of Reduced Dimensions, edited by D. Lockwood and A. Pinczuk (Kluwer, Dordrecht, 1993), p. 221.
[31] J.M. Shi, F.M. Peeters, and J.T. Devreese, Phys. Rev. B **48**, 5202 (1993).
[32] E.P. Pokatilov and M.M. Rusanov, Fiz. Tverd. Tela (Leningrad) **10**, 3117 (1969) [Sov. Phys. Solid State **10**, 2458 (1969)].
[33] D.R. Cohn, D.M. Larsen, and B. Lax, Phys. Rev. B **6**, 1367 (1972).
[34] D.M. Larsen, Phys. Rev. B **6**, 823 (1974).
[35] J.P. Cheng, B.D. McCombe, J.M. Shi, F.M. Peeters, and J.T. Devreese, Phys. Rev. B **48**, 7910 (1993).
[36] H.J. Lee, L.Y. Juravel, J.C. Wolley, and A.J. Springthorpe, Phys. Rev. B **21**, 659 (1980).
[37] S. Adachi, J. Appl. Phys. **58**, R1 (1985).
[38] T. Ando and S. More, Surf. Sci. **113**, 124 (1982).
[39] G. Lindemann, R. Lassnig, W. Seidenbusch, and E. Gornik, Phys. Rev. B **28**, 4693 (1983).
[40] P.M. Platzman, Phys. Rev. **125**, 1961 (1962).
[41] D.M. Larsen, J. Phys. Chem. Solids **29**, 271 (1968).
[42] X.G. Wu, F.M. Peeters, and J.T. Devreese, Phys. Rev. B **40**, 4090 (1989).

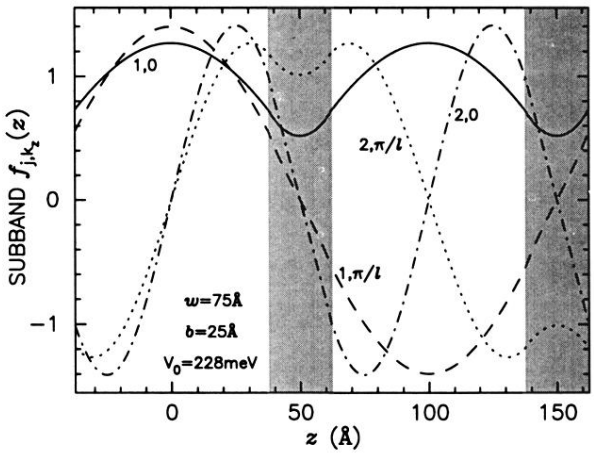

FIG. 1. The subband wave functions corresponding to the energy miniband edges of the two lowest subbands of a $GaAs/Al_{0.3}Ga_{0.7}As$ superlattice with well width $w = 75$ Å and barrier width $b = 25$ Å. The position of the latter is indicated by the shaded area. The lower and the upper edges of the first subband are given by solid and dashed curves, and those of the second subband by dotted and dash-dotted curves, respectively.