D^- states in $GaAs/Al_xGa_{1-x}As$ superlattices in a magnetic field

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(Received 6 October 1993; revised manuscript received 21 December 1994)

The states of a negative donor center (D^-) located at the center of a quantum well of a $GaAs/Al_xGa_{1-x}As$ superlattice are investigated theoretically in a magnetic field applied along the growth axis. The energy levels of the ground (singlet $|1s,1s;s\rangle$) state and four excited (triplet $|1s,2p^{\pm};t\rangle$ states and the singlet $|1s,2p^{\pm};s\rangle$) state of the D^- center are obtained as functions of the magnetic field. The calculation is based on a variational approach in which we use trial wave functions with six variational parameters. We have investigated the influence of the following effects on the energy of the D^- states: (1) tunneling of the electrons into the adjacent wells of the superlattice, (2) electron-electron (e-e) correlation, and (3) the electron-phonon interaction. The magnetopolaron effect on these energies is studied within second-order perturbation theory. A detailed comparison is made between our theoretical results and available experimental data which are interpreted as transition energies between the D^- states. The effect of band nonparabolicity is of minor importance for most of the transition energies except for the transition from the D^- ground state to the $|1s,2p^+;s\rangle$ state at high-magnetic fields.

I. INTRODUCTION

There has been an increasing interest, both experimental and theoretical, in the investigation of quasi-two-dimensional (Q2D) systems, such as semiconductor heterostructures, quantum wells, and superlattices, because of their intrinsic physical interest and their technological applications in electronic devices.[1–3] One of these systems which is very extensively studied is the $GaAs/Al_xGa_{1-x}As$ superlattice. In such a superlattice the difference in the band gap of the two semiconductors acts as an additional periodic square-well potential which confines electrons mainly to the GaAs wells and this influences strongly their physical properties. Quasifree electrons are made present in such systems through, e.g., Si doping. If such dopants are present in a $GaAs/Al_xGa_{1-x}As$ superlattice[4–17] with a very low concentration, electrons will be bound to these shallow donors at low temperatures.

Using selective doping of a $GaAs/Al_xGa_{1-x}As$ superlattice it is possible to realize the situation in which the electrons which are weakly bound to shallow donors in the $Al_xGa_{1-x}As$ barriers $D^0(b)$ are transferred to the GaAs wells where they are trapped by neutral donors $D^0(w)$, forming stable negatively charged donor centers which are referred to as D^- centers. This process can be expressed by

$$D^0(w) + D^0(b) \rightarrow D^-(w) + D^+(b).$$

Such centers are an analogous system to the negative hydrogen ion,[18] which has been extensively studied in astrophysics. In such a system, a hydrogen atom binds an extra electron. This system has attracted considerable attention since the early days of quantum mechanics.[19] D^- centers are one of the simplest "many-body" electronic systems which can be used as a test for theoretical descriptions of e-e correlation. Already many experimental results are available which show the existence of the D^- centers in bulk GaAs (Ref. 20) and in $GaAs/Al_xGa_{1-x}As$ superlattices[13,14,21–25] in the presence of a strong magnetic field. These observations have motivated many theoretical studies.[26–33]

Using the diffusion quantum Monte Carlo approach Pang and Louie[26] studied the ground state of the D^- center in a magnetic field, and obtained the highly accurate energy of the D^- ground state in the absence of electron-phonon interaction. For a strictly two-dimensional (2D) system in a strong magnetic field Larsen and McCann[27] and Dzyubenko[28] independently found that only the ground state and the three lowest triplet states are bound in that limit. This differs from the three-dimensional (3D) case where an infinite number of bound states can be formed in a nonzero magnetic field.[34,35] Xia and Quinn[29] employed the local spin density functional method to calculate the ground state and the lowest triplet states of a D^- center. Dzyubenko and Sivachenko[30] extended the calculation of the D^- center to more excited states. But their calculation is only suitable in the high magnetic-field region. The effect of electron-phonon interaction on the D^- states have been taken into account in Refs. 30–33, where a larger polaron correction to the D^- state is found than to the D^0 state. But all the theoretical investigations of the D^- center mentioned here are limited to a *single*-quantum-well (QW) system with the exception of Ref. 33 where preliminary results were published for a superlattice system.

The binding energy of the D^- center is very small compared to that of the D^0 donor: in the absence of a magnetic field the binding energy of the D^- ground state is only 5.55% (12.8%) of the hydrogenic binding energy in

a 3D (2D) system.[19,26,36] As a consequence the binding energy of the D^- ground state in a Q2D system should be between $0.055\mathcal{R}^*$ and $0.51\mathcal{R}^*$ with $\mathcal{R}^*$ the effective Rydberg. In our previous work on the D^0 center in a superlattice[10] we found that the effect of the adjacent wells in the superlattice is appreciable. For example, at zero magnetic field the binding-energy difference between the D^0 ground state in a GaAs/$Al_{0.3}Ga_{0.7}$As QW with 100 Å well width and the one in a superlattice with 100 Å barrier and 100 Å well widths is more than $0.24R^*$, which is comparable to the binding energy of the D^- center in such a system. At present all the experiments on D^- centers in Q2D systems are done in multiple quantum wells and superlattices. Thus, the QW theory is not a good approximation to explain the binding energies of the D^- centers in superlattices with the exception of superlattices with very thick barriers.

Because GaAs is a polar material the polaron effects on the electronic states of the donor are important, not only at resonance but also at low magnetic fields. This has been extensively investigated by several groups for the cases of bulk GaAs,[37,38] GaAs/Al_xGa_{1-x}As QW's (Refs. 8 and 9) and superlattices.[10] These effects on the D^- center in QW's were discussed in Refs. 30–32 where only the few lowest states were included as intermediate states in the calculation of the polaron correction. Recently, we proved that these calculations seriously underestimate the polaron effects.[33]

In this paper, we present a theoretical study of the D^- center which is located at the quantum-well center of a GaAs/Al_xGa_{1-x}As superlattice in a magnetic field directed along the growth axis. The two electrons in the D^- center are associated with the lowest subband of the superlattice with zero momentum. The energy levels of the lowest five D^- states are the ground state $|1s,1s;s\rangle$, the two lowest triplet states $|1s,2p^{\pm};t\rangle$, and the two lowest-excited singlet states $|1s,2p^{\pm};s\rangle$ are obtained as function of the magnetic-field strength. The calculation is based on a variational approach in which Gaussian type of wave functions[39] is used in combination with additional terms which describe the *e-e* correlation. Since most of the optical experiments on the D^- center were done at high magnetic fields ($B > 4$ T), Gaussian type of wave functions is expected to work well. We compare these results with those with and without the inclusion of *e-e* correlation in the case of a *single*-quantum well approximation. The polaron effects on these levels are included within second-order perturbation theory. We found that this effect is very important in the formation of the D^- centers because it greatly increases the binding energy. A detailed comparison is performed with the available experiment data, especially with those of Huant and co-workers.[13,21] We found that the measurements should be interpreted as being the transition energy between the ground state and the singlet excited state of the D^- center. This was also recently pointed out independently by Larsen and McCann[27] and Dzyubenko.[28] The effect of band nonparabolicity on the transition energy of the D^- center is also discussed by using the standard Kane model,[37] which is found to be important only for the transition $|1s,1s;s\rangle \rightarrow |1s,2p^+;s\rangle$ at high magnetic fields. Our results are in good agreement with the experimental data.

This paper is organized as follows. In Sec. II a variational calculation of the D^- states in a superlattice in a magnetic field is presented in the absence of electron-phonon interaction. The importance of *e-e* correlation and of taking a superlattice versus a QW is investigated. The polaron correction to the energy levels of the D^- center is calculated in Sec. III. A detailed comparison with the available experimental data is performed in Sec. IV. Section V is devoted to our discussions and conclusions.

II. VARIATIONAL APPROACH

A D^- center in a GaAs/Al_xGa_{1-x}As superlattice consists of two electrons which are bound to a positive Si-donor center. This system can be described within the framework of an effective-mass approximation by including (1) the Coulomb potential between the donor ion and the electrons, (2) the *e-e* interaction, and (3) the Fröhlich electron-phonon interaction which describes the dynamical polarization of the lattice due to the electrons. These assumptions are justified for shallow donor centers in compound semiconductors, both 3D and Q2D systems with not too narrow quantum wells, in which the donor radii are much larger than the interatomic distance and the dominant electron-phonon coupling is the Fröhlich coupling with the bulk-GaAs longitudinal-optical (LO-) phonon modes. Such a D^- center located at the well center (which is taken as the origin of our coordinate system) of a GaAs/Al_xGa_{1-x}As superlattice placed in a uniform and constant magnetic field $\vec{B}$ which is directed along the growth axis (taken as the z axis) is described by the Hamiltonian

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

where $H_{e,e}$ is the electronic part

$$H_{e,e} = H_e(\vec{r}_1) + H_e(\vec{r}_2) + H_{1,2}(\vec{r}_1,\vec{r}_2), \tag{2}$$

with $H_e(\vec{r}_j)$ the Hamiltonian for the jth shallow-donor electron given by

$$H_e(\vec{r}_j) = \left(\vec{p}_j + \frac{e}{c}\vec{A}_j\right)\frac{1}{2m_e^*(z_j)}\left(\vec{p}_j + \frac{e}{c}\vec{A}_j\right) - \frac{e^2}{\epsilon_0 r_j} + V(z_j), \tag{3}$$

and $H_{1,2}(\vec{r}_1,\vec{r}_2)$ the Hamiltonian for the Coulombic interaction between the two electrons

$$H_{1,2}(\vec{r}_1,\vec{r}_2) = \frac{e^2}{\epsilon_0 r_{12}}. \tag{4}$$

Equation (3) describes a hydrogenic atom placed in a superlattice in an external magnetic field $\vec{B}$, where $\vec{p}_j$ ($\vec{r}_j$) is the momentum (position) operator of the jth electron, the vector potential $\vec{A}_j$ for the jth electron is defined as

$\vec{A}_j = \frac{1}{2}\vec{B} \times \vec{r}_j$, where we use the symmetrical gauge, c is the velocity of light in vacuum, and $-e$ is the electron charge. The potential of the superlattice in Eq. (3) is modeled by a square-well potential

$$V(z_j) = \begin{cases} 0, & |z_j| < w/2 \\ V_0, & w/2 < z_j < w/2 + b, \end{cases} \tag{5}$$

which is periodically repeated, i.e., $V(z) = V[z+n(w+b)]$ with w the well width, b the barrier width, and n an integer. For a $GaAs/Al_xGa_{1-x}As$ interface the barrier height V_0 is given by 60% of the total energy-band-gap difference between the two semiconductors: $\Delta E_g = 1.155x + 0.37x^2$ eV.[40] $r_j = (\rho_j^2 + z_j^2)^{1/2}$ is the distance between the jth electron and the donor center, $\rho_j = (x_j^2 + y_j^2)^{1/2}$ is the distance in the x-y plane, and $r_{12} = |\vec{r}_1 - \vec{r}_2|$ is the distance between the two electrons. The quantity $m_e^*(z_j)$ is the effective mass of the jth electron, which is different in the two semiconductors: in the GaAs wells $m_w/m_e = 0.067$, and in the $Al_xGa_{1-x}As$ barriers $m_b/m_e = 0.067 + 0.083x$.[41] $\epsilon_0 = 12.5$ is the static dielectric constant of GaAs,[41] which is assumed to be the same in both materials. In optical experiments on D^- centers electronic transitions are induced without a spin flip, and consequently we do not have to include the term

$$H_{\rm spin} = \sum_{j=1}^{2} \frac{m_w}{2m_e^*(z_j)} g^* \mu_B \vec{B} \cdot \vec{\sigma}_j$$

in Eq. (2), where $\mu_B = e\hbar/2m_w c$ is the Bohr magneton in GaAs, g^* the gyromagnetic (g) factor, and $\vec{\sigma}_j$ is the Pauli matrices of the jth electron.

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

$$H_{\rm LO} = \sum_{\vec{q}} \hbar\omega_{\vec{q}} \left(a_{\vec{q}}^\dagger a_{\vec{q}} + \frac{1}{2} \right), \tag{6}$$

where $a_{\vec{q}}^\dagger$ ($a_{\vec{q}}$) is the creation (annihilation) operator of a LO phonon with wave vector $\vec{q}$ and frequency $\omega_{\vec{q}}$. For GaAs we take $\hbar\omega_{\vec{q}} = \hbar\omega_{\rm LO} = 36.75$ meV,[37] the value of the LO-phonon energy at 4.2 K, which is the temperature region in which the magneto-optical experiments on the D^- center have been performed.

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

$$H_I = \sum_{\vec{q}} [V_{\vec{q}}\, a_{\vec{q}} (e^{i\vec{q}\cdot\vec{r}_1} + e^{i\vec{q}\cdot\vec{r}_2}) + V_{\vec{q}}^*\, a_{\vec{q}}^\dagger (e^{-i\vec{q}\cdot\vec{r}_1} + e^{-i\vec{q}\cdot\vec{r}_2})], \tag{7}$$

where $V_{\vec{q}}$ is the Fourier coefficient of the electron-phonon interaction given by

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

with Ω the crystal 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 the material. In our calculation, we take $\alpha = 0.068$ for GaAs,[41] which is a good approximation for the case of a superlattice with not too narrow quantum wells because most of the weight of the electron wave function is confined to the wells. Furthermore, only the interaction with the 3D-bulk GaAs phonon modes is taken into account, and in so doing the effect of the superlattice structure on the phonon modes is neglected. In a previous work,[42] we have found that this is a good approximation for the case of $GaAs/Al_xGa_{1-x}As$ systems.

Due to the special symmetry of our problem it is convenient to introduce cylindrical polar coordinates (ρ, ϕ, z) with the z direction oriented along the growth axis. The electronic Hamiltonians H_e and $H_{1,2}$ reduce to the following forms:

$$H_e(\vec{r}_j) = -\frac{m_w}{m_e^*(z_j)} \left(\nabla_j^2 - \gamma L_{z_j} - \frac{1}{4}\gamma^2\rho_j^2 \right) - \frac{2}{r_j} + V(z_j), \tag{8}$$

and

$$H_{1,2}(\vec{r}_1, \vec{r}_2) = \frac{2}{r_{12}}, \tag{9}$$

where we have also introduced the effective Bohr radius $a_0^* = \hbar^2\epsilon_0/m_w e^2 = 98.7$ Å as the unit of length, the effective Rydberg $\mathcal{R}^* = e^2/2\epsilon_0 a_0^* = 5.83$ meV as the unit of energy, and $\gamma = e\hbar B/2m_w c\mathcal{R} = 0.148B$ (T) as the dimensionless unit of the magnetic-field strength, and $L_z = -i(\partial/\partial\phi)$ is the z component of the angular momentum operator in units of $\hbar$ which is still a good quantum number.

The Schrödinger equation with the Hamiltonian $H_{e,e}$ cannot be solved exactly, and therefore we rely on a variational approach for the wave functions and the energy levels of the D^- states. We will study the ground state $|1s, 1s; s\rangle$, the triplet states $|1s, 2p^\pm; t\rangle$, and the singlet states $|1s, 2p^\pm; s\rangle$. In the present work, we have neglected all interactions involving the spin of the electrons (spin-orbit, spin-spin). The total wave function Φ of the D^- state can be written as the product of the space wave function $\Psi(\vec{r}_1, \vec{r}_2)$ and the spin wave function $\chi(1,2)$

$$\Phi = \Psi(\vec{r}_1, \vec{r}_2)\chi(1,2). \tag{10}$$

Since Φ must be *antisymmetric*, the product function Eq. (10) has to consist of an antisymmetric function and a symmetric function: either the spatial part is symmetric [i.e., $\Psi(\vec{r}_1, \vec{r}_2) = \Psi(\vec{r}_2, \vec{r}_1)$] and the spin part is antisymmetric [i.e., $\chi(1,2) = -\chi(2,1)$], or vice versa. As is well known, the spin wave function is of a particularly simple nature: for each electron only two possible eigenvalues of the z component of the spin-vector operator are found $+\frac{1}{2}$ or $-\frac{1}{2}$. Therefore, in a D^- center the two electrons have four independent spin configurations: one is antisymmetric ($S = 0$, the absolute value of the total spin), and the other three are symmetric ($S = 1$). A D^- state

with a symmetric spatial wave function is a *singlet* state with *one* antisymmetric spin wave function, while the one with an antisymmetric spatial wave function is a *triplet* state which can have *three* different symmetric spin wave functions ($S_z = 0, \pm 1$). In the following, we will concentrate on the spatial parts of the wave functions only.

A Chandrasekhar-type trail wave function[43] is adopted for the spatial part of the wave function of the D^- state with the following general structure:

$$\Psi_{I,O;\Lambda}(\vec{r}_1,\vec{r}_2) = [\psi_I(\vec{r}_1)\psi_O(\vec{r}_2) + \Lambda\psi_O(\vec{r}_1)\psi_I(\vec{r}_2)] \times[1 + \Theta_{I,O;\Lambda}(z_1 - z_2)^2 + \Xi_{I,O;\Lambda}(\rho_1 - \rho_2)^2], \quad (11)$$

where $I(O)$ indicates the inner (outer) orbitals ψ_I (ψ_O), and Λ is an index describing the symmetry of the wave function under exchange of the two electrons: $\Lambda = s = +1$ corresponds to the singlet states, and $\Lambda = t = -1$ corresponds to the triplet states. In our calculation the inner orbitals $\psi_I(\vec{r})$ are always chosen to have the same functional form as the donor (D^0) ground state, and the outer orbitals $\psi_O(\vec{r})$ vary depending on the states: for the D^- ground state ($\Psi_{1s,1s;s}$) it has the same functional form as $\psi_I(\vec{r})$ (although with different variational parameters), and for the excited states they will have a functional form similar to the $2p^+$ or $2p^-$ states of the D^0 center. Thus, following Ref. 10, $\psi_\kappa(\vec{r})$ ($\kappa = I, O$) are taken to be $\psi_\kappa(\vec{r}) = f(z)\rho^{|m_\kappa|}\exp(im_\kappa\phi - \xi_\kappa\rho^2 - \eta_\kappa z^2)$, where m_κ is the magnetic quantum number of the electron, ξ_κ and η_κ are the variational parameters which depend on both the magnetic field and the structure of the system, and $f(z)$ is the wave function which is the lowest-energy ($E_{z,1}$) solution of the superlattice potential Eq. (5) with the property $f(z) = f[z + n(w + b)]$. The explicit form of $f(z)$ can be found in many papers, e.g., Ref. 10. The *e-e* correlation in the D^- state is described by the polarization terms, i.e., $\Theta_{I,O;\Lambda}(z_1 - z_2)^2$ and $\Xi_{I,O;\Lambda}(\rho_1 - \rho_2)^2$ in Eq. (11). In a 3D system, the correlation factor is crucial since it contributes about half of the binding energy of the D^- ground state.[19]

In the absence of the electron-phonon interaction the energy expectation value of the D^- state Ψ_μ [$\mu = (I, O; \Lambda)$] is given by the following equation

$$E^0_\mu = \frac{\langle\Psi_\mu|H_{e,e}|\Psi_\mu\rangle}{\langle\Psi_\mu|\Psi_\mu\rangle}, \quad (12)$$

which we minimize numerically with respect to the six variational parameters: Θ_μ, Ξ_μ, ξ_I, η_I, ξ_O, and η_O, and this for each state.

Figure 1 shows the extent of the wave functions in the direction perpendicular to the growth axis for the outer and inner electrons of the ground state (solid curves) and the triplet state (dashed curves) of the D^- center in an $x = 0.25$, $w = 100$ Å QW as a function of the magnetic field. The corresponding results for the $1s$ and $2p$ states of the D^0 center (dash-dotted curves) (Ref. 10) and for a free electron (i.e., $2a_0^*/\sqrt{\gamma}$) are also plotted for comparison. Notice the following: (1) the inner orbitals of the D^- center in the x-y plane have almost the same extension (although a little smaller) and the same dependence on the magnetic field as the $1s$-electron wave function of the shallow donor. However, the extension of the outer orbitals is close to that of the free electron when $\gamma > 1$, but are more extended than the $2p$ orbital of the D^0 state; (2) the orbitals which are more spread out at zero magnetic field have a stronger dependence on the magnetic field; and (3) the outer electron of the triplet state is always more spread out than that of a free electron. At low magnetic fields it also extends to infinity at $\gamma = 0$.

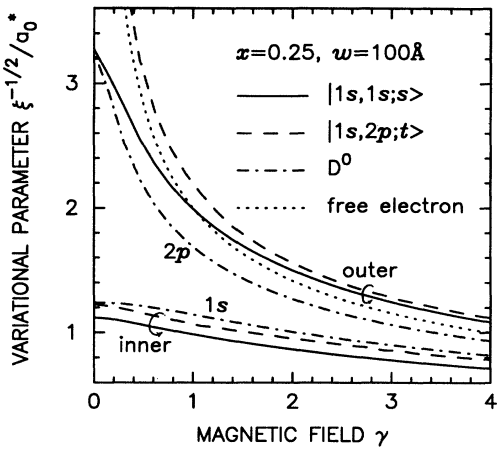

FIG. 1. The extent (in units of $a_0^* = 98.7$ Å) of the electron wave function in the x-y plane for the D^- and D^0 centers at the well center of a GaAs/$Al_{0.25}Ga_{0.75}$As QW with $w = 100$ Å as a function of magnetic field γ. Solid curves are for the outer and inner electrons in the D^- ground state, dashed curves for those in the D^- triplet state, dash-dotted curves for the D^0 ground state, and dotted curves for the D^0 $2p$-like state. As a comparison, the extent of a free electron ($2a_0^*/\gamma^{1/2}$) is also shown (the dotted curve).

In our previous work,[10] we have found that the difference of the binding energy for the D^0 ground state in a $w = b = 100$ Å superlattice and a $w = 100$ Å QW in the absence of any magnetic field is about $0.24\mathcal{R}^*$, which is comparable to the largest binding energy of a D^- center in the Q2D system. In Fig. 2 we present the binding energy of the three D^- states, $|1s, 1s; s\rangle$, $|1s, 2p; t\rangle$, and $|1s, 2p; s\rangle$, as a function of the magnetic field in a superlattice with $x = 0.25$, and $w = b = 100$ Å (solid curves). These results are compared to the corresponding results (dashed curves) in an $x = 0.25, w = 100$ Å QW, and also to the results (dotted curves) in the same QW but for the variational approach used in Ref. 30 where the effect of *e-e* correlation was not included, and which resulted in the energy level E^0_μ(n.c.) for the D^- μth state. Note that the binding energy of the D^- center is defined as the minimum energy which is required to remove one electron to infinity and the final state is a D^0 center in the ground state and a free electron. In this process, the electron spin configuration is not changed. Consequently, the binding energy of the D^- μth state can be expressed by

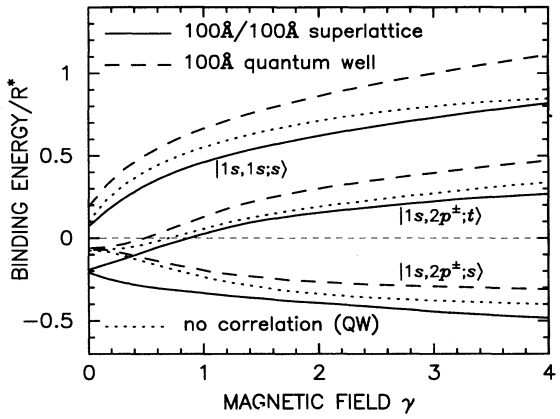

FIG. 2. Binding energies (in units of $\mathcal{R} = 5.83$ meV) of the ground state, the triplet state, and the lowest singlet excited state for the D^- center at the well center of a $GaAs/Al_{0.25}Ga_{0.75}As$ superlattice with $w = b = 100$ Å (solid curves) as a function of magnetic field. The corresponding results for the QW with (dashed curves) and without (dotted curves) electron-electron correlation are also plotted. The thin dashed line indicates zero value of the binding energy.

$$E_\mu^b = E_{1s}^0(D^0) + E_{z,1} + \left(N + \frac{1}{2}\right)\hbar\omega_c A - E_\mu^0, \quad (13)$$

where $E_{1s}^0(D^0)$ is the energy of the D^0 ground state. A detailed description of this state has been given in Ref. 10. In Eq. (13) $\omega_c = eB/m_w c$ is the cyclotron resonance frequency for a noninteracting electron in GaAs, and N is the Landau level quantum number: $N = 1$ for the states with magnetic quantum number $m_o = +1$, otherwise $N = 0$. A factor of $A = \langle f(z)|m_w/m_e^*(z)|f(z)\rangle/\langle f(z)|f(z)\rangle$ appears in Eq. (13) which is a consequence of the electronic mass discontinuity at the interfaces of GaAs and $Al_xGa_{1-x}As$. From this figure we find that (1) the binding energies of the ground state and the triplet state are an increasing function of the magnetic field, and the $|1s,1s;s\rangle$ state is always bound (i.e., above the thin dashed line which indicates $E^b = 0$) while the $|1s,2p;t\rangle$ state becomes bound for $\gamma > 0.5$ in the QW case and $\gamma > 0.8$ in the superlattice case; (2) an opposite B dependence is found for the singlet excited state $|1s,2p;s\rangle$ which is always unbound (i.e., below the thin dashed line); (3) the binding energy in the superlattice case is appreciably decreased as compared to that of the QW case, which shows that the QW theory is not a good approximation for the calculation of the binding energy of the D^- center in this type of superlattices; (4) e-e correlation increases the binding energy of the D^- center appreciably which is similar to the case of a 3D system.[19] This effect is more important for the lower states and at higher magnetic fields. This is a result of the fact that in both cases the electron states are more localized (see Fig. 1), and consequently the e-e correlation terms will contribute more to the wave functions.

The actual energy difference $E_\mu^0(\text{n.c.}) - E_\mu^0$ between the two variational approaches with and without the e-e correlation terms in the wave functions is plotted in Fig. 3(a) as a function of the magnetic field for the D^- states in the same QW as shown in Fig. 1. It is clear that for all the states the energy difference monotonously increases with increasing magnetic fields. This difference for the ground state has an almost constant slope, while for the excited states it increases much more rapidly than for the ground state in low magnetic fields ($\gamma < 1.5$), and much less rapidly in high magnetic fields. The relative percentage contribution from e-e correlation is given in Fig. 3(b), which indicates that (1) the e-e correlation is more important for the ground state than for the excited state and (2) this correlation in the ground state increases with increasing magnetic fields, while in the excited state it increases at low magnetic fields ($\gamma < 2$) and decreases slightly in the high magnetic field region.

Now we will describe another method to investigate the importance of correlation in the D^- states. In the wave function of the μth state of the D^- center the e-e correlation is connected by the variational parameters Θ_μ and Ξ_μ in Eq. (11). Thus, the correlation energy of the D^- state can also be defined through the difference

$$[\langle\Psi_\mu(\Theta_\mu,\Xi_\mu)|H_{e,e}|\Psi_\mu(\Theta_\mu,\Xi_\mu)\rangle - \langle\Psi_\mu(0,0)|H_{e,e}|\Psi_\mu(0,0)\rangle]/\langle\Psi_\mu(\Theta_\mu,\Xi_\mu)|\Psi_\mu(\Theta_\mu,\Xi_\mu)\rangle\,.$$

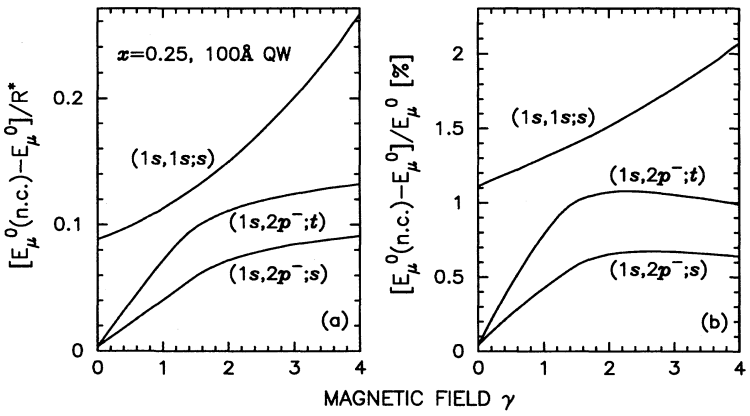

FIG. 3. In (a) the energy difference $E_\mu^0(\text{n.c.}) - E_\mu^0$ between the two variational approaches with (E_μ^0) and without [E_μ^0(n.c.)] e-e correlation is shown as a function of the magnetic field for a D^- center in a QW with $x = 0.25$ and $w = 100$ Å; and in (b) the relative percentage of this difference is plotted.

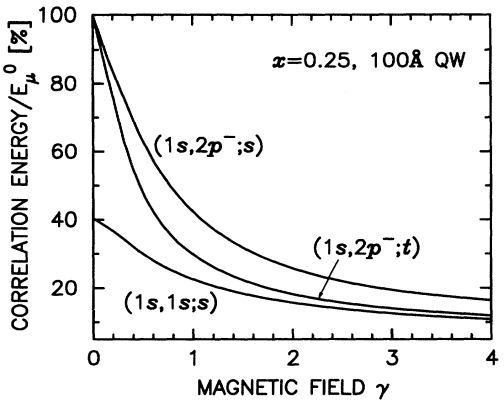

FIG. 4. Percentage of the correlation contribution to the energy of the $(1s,1s;s)$, $(1s,2p^-;t)$, and $(1s,2p^-;s)$ states as a function of the magnetic field for a D^- center in a QW with $x = 0.25$ and $w = 100$ Å.

This difference scaled with the energy of the different D^- states is shown in Fig. 4 for $\mu = (1s,1s;s)$, $(1s,2p^-;t)$, and $(1s,2p^-;s)$ as a function of the magnetic field for a D^-center in an $x = 0.25$, $w = 100$ Å QW. Notice that (1) the relative contribution of the correlation terms to the energy of all the D^- states decreases with increasing magnetic fields. The reason is that the magnetic field forces the electrons closer to the donor center, thus the Coulomb energy between the electrons and the donor ion increases, and this leads to the rapid decrease of the wave function of the D^- electrons. As a consequence, the correlation terms which favor large values of $|z_1 - z_2|$ and/or $|\rho_1 - \rho_2|$ becomes less important than those in a lower-magnetic field; (2) in the absence of a magnetic field the correlation energy is about 40% of the energy of the D^- ground state, while it is almost 100% of the energy for both excited states; and (3) the correlation contribution to a D^- state which is more spread out is more sensitive to the magnetic field.

From a first glance the differences between Fig. 3(b) and Fig. 4 are remarkable. Not only are the absolute values more than an order of magnitude different but also the relative positions of the different curves are different. But we should keep in mind that the subtraction of the correlation energy in Fig. 3(b) and Fig. 4 are obtained in two total different manners. In Fig. 3(b) the energies E_μ^0(n.c.) and E_μ^0 are given from two different variational calculations with a different number of variational parameters, while in Fig. 4 the correlation terms in the energy are subtracted out within one variational calculation using the same wave-function normalization $\langle\Psi_\mu(\Theta_\mu,\Xi_\mu)|\Psi_\mu(\Theta_\mu,\Xi_\mu)\rangle$.

III. POLARON CORRECTION

In the calculation of the polaron correction to the electronic states it is a good approximation to include only GaAs bulk-phonon modes for superlattices or QW's with not too narrow wells.[10,44,45] Therefore, the electron-phonon interaction for a D^- center will be described by the Fröhlich Hamiltonian given by Eq. (7). Since GaAs is a weakly polar material with electron-phonon coupling constant $\alpha = 0.068$, which is much smaller than 1, we can use second-order perturbation theory to calculate the polaron correction to the energy of the μth state of the D^- center

$$\Delta E_\mu = -\sum_{\mu'}\sum_{\vec{q}} \frac{|\langle\mu';\vec{q}|H_I|\mu;\vec{0}\rangle|^2}{\hbar\omega_{\rm LO} + E^0_{\mu'} - E^0_\mu - \Delta_\mu}, \tag{14}$$

where $\Delta_\mu = 0$ for all states in the polaron nonresonant region, which corresponds to Rayleigh-Schrödinger perturbation theory. For the $|1s,2p^+;s\rangle$ state we take $\Delta_{1s,2p^+;s} = \Delta E_{1s,2p^+;s} - \Delta E_{1s,1s;s}$, which corresponds to improved Wigner-Brillouin-perturbation theory.[46,47] In Eq. (14) $|\Psi_{\mu'};\vec{q}\rangle$ describes a D^- state composed of two electrons with unperturbed energy $E^0_{\mu'}$ and a LO phonon with momentum $\hbar\vec{q} = \hbar(\vec{q}_\parallel, q_z)$ and energy $\hbar\omega_{\vec{q}}$. Because the spin configuration of the triplet states are orthogonal to the one of the singlet states, they do not contribute to the polaron correction of the singlet states, and vice versa. Because of the property of identical electrons we have the symmetry relation: $\Psi_\mu(\vec{r}_1,\vec{r}_2) = \pm\Psi_\mu(\vec{r}_2,\vec{r}_1)$ which implies that Eq. (14) can be written as

$$\Delta E_\mu = -4\sum_{\mu'}\sum_{\vec{q}} \frac{|V_{\vec{q}}|^2|\langle\Psi_{\mu'}|e^{-i\vec{q}\cdot\vec{r}_1}|\Psi_\mu\rangle|^2}{\hbar\omega_{\rm LO} + E^0_{\mu'} - E^0_\mu - \Delta_\mu}. \tag{15}$$

In order to obtain the polaron correction to the D^- energy of the μth state, one has to sum over *all* the D^- states in Eq. (14) whose spin configurations have the same symmetry as that of the μth state. This is a formidable task. In Refs. 30–32, only a finite number of states were included in the sum $\sum_{\mu'}$. Recently,[33,38] we found that in the nonresonant magnetic-field region such an approach is unsatisfactory and underestimates the polaron correction appreciably. Nevertheless, it is possible to evaluate Eq. (15) approximately in such a way that one needs to know only a few relevant states.[48,38] Using the method of Ref. 48 one can rewrite Eq. (15) into three parts: the first is the *leading term*, $-4\alpha\hbar\omega_{\rm LO}$, which is the polaron energy of a free bipolaron in a 3D system in the absence of any fields;[49] the second term is small, and in fact is equal to zero in the approximation of $m_w = m_b$, which will be assumed when we calculate the polaron correction; and the third term contains a sum over all the D^- states. Thus, Eq. (15) can be reduced to the result given by

$$\Delta E_\mu = -4\alpha\hbar\omega_{\rm LO} - 4\sum_{\mu'}\sum_{\vec{q}} \frac{|V_{\vec{q}}|^2|\langle\Psi_{\mu'}|e^{-i\vec{q}\cdot\vec{r}_1}|\Psi_\mu\rangle|^2(E^0_{\mu'} - E^0_\mu - q^2 - \Delta_\mu)^2}{(\hbar\omega_{\rm LO} + E^0_{\mu'} - E^0_\mu - \Delta_\mu)(\hbar\omega_{\rm LO} + q^2)^2}. \tag{16}$$

The calculation of the polaron correction to the energy of the D^- state is now reduced to evaluate the second term on the right-hand side of Eq. (16). Recently, we gave a very detailed discussion[38] on the polaron correc-

tion to the energy levels of a D^0 center in bulk GaAs, where the different approximations were discussed in order to obtain the polaron correction in the resonant and in the nonresonant region. Following this approach for the nonresonant states, e.g., the ground state $|1s,1s;s\rangle$ and the $|1s,2p^-;s\rangle$ state, we obtain

$$\Delta E_\mu = -4\alpha(\hbar\omega_{\rm LO} + Y_\mu), \tag{17}$$

where $Y_\mu = \frac{1}{6}\langle\Psi_\mu|[H_e(\vec{r}_1) - V(z_1) + 2/r_1]|\Psi_\mu\rangle/\langle\Psi_\mu|\Psi_\mu\rangle$. The factor of $\frac{1}{6}$ obtained here[50] has been proven to be an improvement to the factor of $\frac{2}{3}$ (Refs. 48 and 38) which gives a rigorous upper bound to the polaron correction to the ground state of the donors. For the excited state $|1s,2p^+;s\rangle$, there may exist another μth state of the D^- center such that at higher magnetic fields we have $E^0_{1s,2p^+;s} \sim E^0_\mu + \hbar\omega_{\rm LO}$. Consequently, this μth state will give the dominant contribution to the sum $\sum_{\mu'}$ in Eq. (16). Therefore, near resonance it is sufficient to limit the sum $\sum_{\mu'}$ to such states. In the present work, we have included the ground state and the two lowest excited states in the sum $\sum_{\mu'}$. However, in order to obtain also reliable results in the polaron nonresonant region, we follow the same approach[38] as for the $2p^+$ state of the D^0 center, and propose the following improved expression for the polaron correction to the $|1s,2p^+;s\rangle$ state

$$\Delta E_{1s,2p^+;s} = \Delta E_{1s,2p^-;s} - 4\sum_{\kappa=2p^\pm}\sum_{\mu'}\sum_{\vec{q}} \frac{m_\kappa |V_{\vec{q}}|^2 |\langle\Psi_{\mu'}|e^{-i\vec{q}\cdot\vec{r}_1}|\Psi_{1s,\kappa;s}\rangle|^2 (E^0_{\mu'} - E^0_{1s,\kappa;s} - q^2)^2}{(\hbar\omega_{\rm LO} + E^0_{\mu'} - E^0_{1s,\kappa;s} - \Delta_{1s,\kappa;s})(\hbar\omega_{\rm LO} + q^2)^2}, \tag{18}$$

where m_κ is the magnetic quantum number of the outer electron with $m_{2p^\pm} = \pm 1$. This expression (18) has the following properties: (1) at $\gamma = 0$ the polaron correction to the $|1s,2p^+;s\rangle$ state is identical to the one of the $|1s,2p^-;s\rangle$ state, which is due to the fact that in this limit both states are identical; (2) for $\gamma > 0$ $|\Delta E_{1s,2p^+;s}|$ is larger than $|\Delta E_{1s,2p^-;s}|$ 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 the second term on the right-hand side of Eq. (18) dominates, which gives the correct resonant positions.

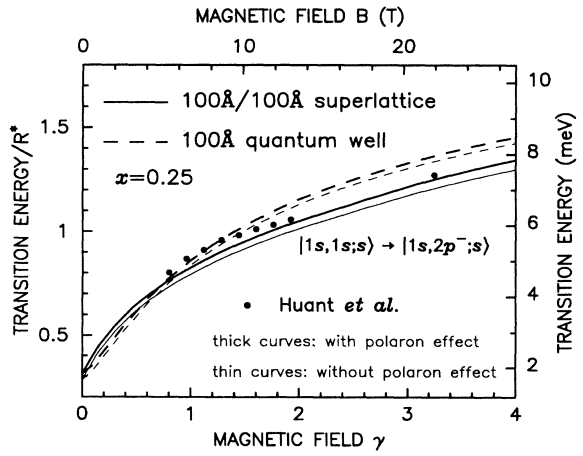

FIG. 5. Transition energy of $|1s,1s;s\rangle \rightarrow |1s,2p^-;s\rangle$ as a function of the magnetic field for a D^- center in a $GaAs/Al_{0.25}Ga_{0.75}As$ superlattice with $w = b = 100$ Å, with (thick solid curve) and without (thin solid curve) polaron correction. The experimental data (solid dots) are from Refs. 21. The corresponding results for a QW (dashed curves) are also plotted.

IV. COMPARISON WITH EXPERIMENTS

At present, there exist several experimental results[13,14,21–25] on the magnetic-field dependence of D^- transitions in $GaAs/Al_xGa_{1-x}As$ superlattices. In a magneto-optical experiment on the D^- center no spin reversal is possible, and thus the $|1s,1s;s\rangle \rightarrow |1s,2p^\pm;t\rangle$ transitions are forbidden. Therefore, the $|1s,2p^-;t\rangle$ state can be considered as another "ground state," from which an independent set of transitions can be obtained. Initially, the experimental results of Huant and co-workers[13,21] were interpreted as transitions from the D^- ground state to a D^0 ground state plus a free electron in the Nth Landau level. Recently, it was argued in Refs. 27 and 28 that experimentally one observed the transition to the singlet excited state of the D^- center. Due to the discreteness of all D^- states in a Q2D system in the presence of a perpendicular magnetic field, the latter transition has the largest oscillator strength. In the present work, we are able to shed some light on this controversy.

The $|1s,1s;s\rangle \rightarrow |1s,2p^-;s\rangle$ transition energy of the D^- center in an $x = 0.25$, $w = b = 100$ Å superlattice is depicted in Fig. 5 with (thick curves) and without (thin curves) polaron correction. The solid dots are the experimental data of Huant, Najda, and Etienne.[21] A reasonable agreement is found between experiment and theory for the superlattice case when we include the polaron effect. Note also that the transition energies for a QW do not agree with experiment and in particular the slope of the curve differs appreciably. This slope is consistent with the results from the variational quantum Monte Carlo calculation.[22] A small polaron correction to the transition energy is obtained due to the fact that the large polaron corrections to the energy levels of both D^- states cancel each other. The polaron effect slightly increases the transition energy because of the larger polaron correction to the ground state as compared to the $|1s,2p^-;s\rangle$ state. In the small magnetic field region the agreement between theory and experiment is less satis-

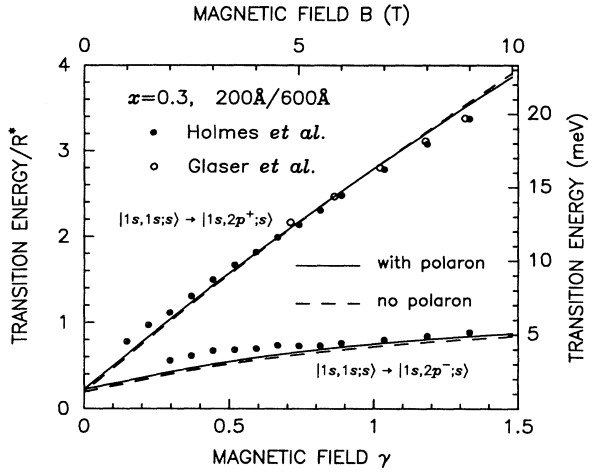

FIG. 6. Transition energy of $|1s,1s;s\rangle \rightarrow |1s,2p^{\pm};s\rangle$ as a function of the magnetic field for a D^- center in a $GaAs/Al_{0.3}Ga_{0.7}As$ superlattice with $w = 200$ Å, $b = 600$ Å with (solid curves) and without (dashed curves) polaron correction. The experimental data (solid circles) are from Ref. 24. The open circles are the measured results from the similar superlattice but $b = 200$ Å by Glaser *et al.* (Ref. 14).

factory, which we think is due to the fact that at small magnetic fields the wave functions should be of exponential type rather than Gaussian type.

Recently, Holmes *et al.*[24] measured the transition energies between the $|1s,1s;s\rangle$ state and the $|1s,2p^{\pm};s\rangle$ states for the D^- center in a $GaAs/Al_{0.3}Ga_{0.7}Al$ superlattice with well width $w = 200$ Å and barrier width $b = 600$ Å in the low magnetic field region ($B \leq 9$ T). In this magnetic-field region, there is no strong polaron resonance. Holmes *et al.*[24] have pointed out that their results could not be explained as being the transition between the D^- state and the $(D^0 + e)$ state. We show in Fig. 6 our theoretical results with (solid curves) and without (dashed curves) electron-phonon interaction together with these experimental data (solid circles). As a comparison, the early experimental results of Glaser *et al.*[14] for the $|1s,1s;s\rangle \rightarrow |1s,2p^{+};s\rangle$ transition are also given by the open circles, which are very close to the results of Holmes *et al.* because a similar sample was used but a thinner barrier, i.e., $b = 200$ Å. Both the $|1s,1s;s\rangle \rightarrow |1s,2p^{-};s\rangle$ and the $|1s,1s;s\rangle \rightarrow |1s,2p^{+};s\rangle$ transition energies of the calculation are in good agreement with the experimental results. As was already shown in Fig. 5, the polaron effect is very important to correctly describe the experimental data for the transition $|1s,1s;s\rangle \rightarrow |1s,2p^{-};s\rangle$ because it shifts the transition energies to higher energies. For $|1s,1s;s\rangle \rightarrow |1s,2p^{+};s\rangle$, it increases the transition energies at low magnetic fields ($\gamma < 0.9$), and it decreases them at higher-magnetic fields ($\gamma > 1.0$). Also here, the theory slightly underestimates the transition energy for $\gamma < 0.8$, which we attribute to the use of Gaussian type of wave functions.

In early work Huant *et al.*[13] studied the optical transitions of shallow donors, and found some lines which at that time could not be completely accounted for. They were tentatively explained as due to D^- transitions. Here we will give a quantitative explanation of their experiment results in an $x = 0.25$, $w = b = 100$ Å superlattice in magnetic fields up to 16 T, which are given in Fig. 7 by the open circles together with the results of Fig. 5 which were obtained from the same superlattice. More recently, Cheng, McCombe, and Schaff[25] have observed a two-level resonance of the $|1s,1s;s\rangle \rightarrow |1s,2p^{+};s\rangle$ transition, whose experimental results are also shown by the solid dots in this figure which are a little higher than those of Huant *et al.* The reason is that a superlattice was used in Ref. 25 with $x = 0.3$, $w = 100$ Å, and $b = 600$ Å, which is more like a QW. Our theoretical results without polaron correction (thin dashed curves) are not able to explain the experiments at high magnetic fields. Including the polaron effect (dotted curves) improves our results appreciably and confirms that the higher branch of the measured $|1s,1s;s\rangle \rightarrow |1s,2p^{+};s\rangle$ transition energies is due to resonance between the $|1s,1s;s;\vec{q}\rangle$ and $|1s,2p^{+};s;\vec{0}\rangle$ states. A larger polaron splitting (about $1.2R^*$) is found in comparison with that (about $0.8R^*$) of the D^0 center,[51] which is consistent with the recent theoretical results of Ref. 30 for an $x = 0.3$, $w = 100$ Å QW, which are shown by the thin dash-dotted curve in the high magnetic-field region. A three-level resonance is found in our calculation since only three D^- states are included in the sum $\sum_{\mu'}$ in Eq. (18). However, at high magnetic fields for the $|1s,1s;s\rangle \rightarrow |1s,2p^{+};s\rangle$ transition the agreement is less satisfactory. Recently, Dzyubenko and Sivachenko[30] have found that band nonparabolicity

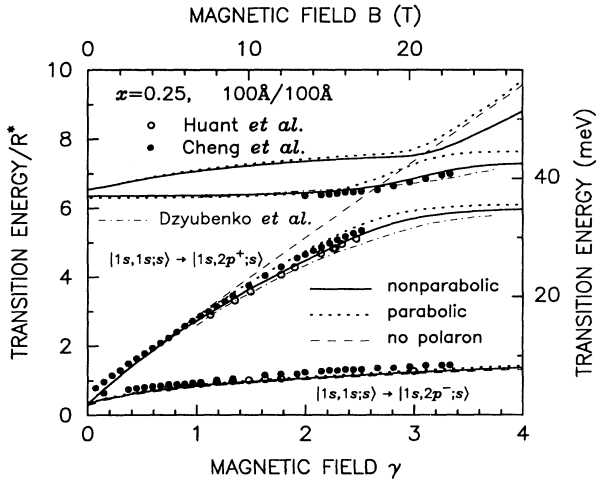

FIG. 7. Transition energy of $|1s,1s;s\rangle \rightarrow |1s,2p^{\pm};s\rangle$ as a function of the magnetic field for a D^- center at the well center of a $GaAs/Al_{0.25}Ga_{0.75}As$ superlattice with $w = b = 100$ Å. The theoretical results are given for the following cases: (1) without polaron correction (thin dashed curves), (2) with polaron effect (dotted curves), and (3) including the effects of polaron and band nonparabolicity (solid curves). The experimental data (open circles) are from Huant and co-workers (Refs. 13 and 21). The solid dots are the experimental results from an $x = 0.3$, $w = 100$ Å, and $b = 600$ Å superlattice of Ref. 25. The thin dash-dotted curve is the theoretical results from Ref. 30.

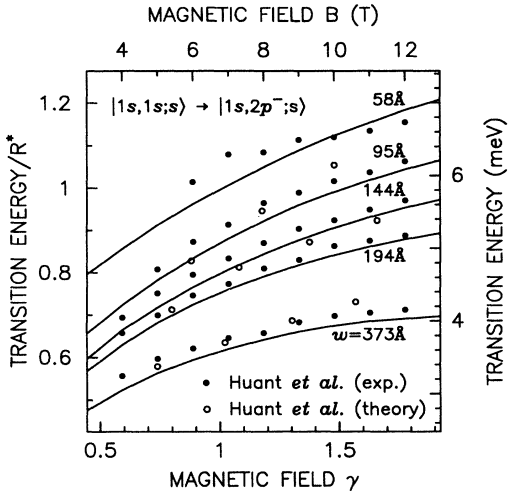

FIG. 8. Energy of the $|1s,1s;s\rangle \rightarrow |1s,2p^-;s\rangle$ transition for a D^- system at the center of the quantum well of a $GaAs/Al_xGa_{1-x}As$ superlattice. Results for the following superlattices are depicted: (1) $w = 58$ Å, $b = 191$ Å, $x = 0.25$; (2) $w = 95$ Å, $b = 194$ Å, $x = 0.26$; (3) $w = 144$ Å, $b = 187$ Å, $x = 0.23$; (4) $w = 194$ Å, $b = 196$ Å, $x = 0.26$; and (5) $w = 373$ Å, $b = 191$ Å, $x = 0.26$. The theoretical results (solid curves) include the effects of polaron and band nonparabolicity. The measured data (solid dots) and the theoretical results (open circles) are from Ref. 22.

changes the magnitude of the D^- transition appreciably. This is different from the binding-energy case, where this effect was found to be negligible.[26,31] We used the standard Kane model given by

$$E_{np} = \frac{E_g}{2}\left(-1+\sqrt{1+\frac{4E_p}{E_g}}\right), \tag{19}$$

to describe band nonparabolicity, which has been successfully applied to describe the effect of band nonparabolicity on the D^0 centers in GaAs (Ref. 38) and in $GaAs/Al_xGa_{1-x}As$ superlattices.[51] In Eq. (19) E_{np} and E_p are the *single*-electron energies with and without the effect of band nonparabolicity, respectively, and $E_g = 1520$ meV is the energy gap of GaAs. For any one of the two electrons in the D^- center, there is no well-defined single electron energy. Therefore, we assign half of the total energy of the D^- state to each electron. This results in the solid curves as depicted in Fig. 7, which show that the effect of the band nonparabolicity slightly decreases the transition energy of the D^- center, and it becomes important only for the $|1s,1s;s\rangle \rightarrow |1s,2p^+;s\rangle$ transition near the resonance. We observe that with this correction our results improve at low-magnetic fields ($\gamma < 2$), but much more for the $|1s,1s;s\rangle \rightarrow |1s,2p^+;s\rangle$ transition energies at high magnetic fields, which leads to a quite good agreement with the experimental data.

More recently, Huant *et al.*[22] performed a series of magneto-optical experiments on D^- centers in different $GaAs/Al_xGa_{1-x}As$ superlattices: (1) $w = 58$ Å, $b = 191$ Å, $x = 0.25$; (2) $w = 95$ Å, $b = 194$ Å, $x = 0.26$; (3) $w = 144$ Å, $b = 187$ Å, $x = 0.23$; (4) $w = 194$ Å, $b = 196$ Å, $x = 0.26$; and (5) $w = 373$ Å, $b = 191$ Å, $x = 0.26$. These data are shown in Fig. 8 by the solid dots together with our theoretical results (curves) of the $|1s,1s;s\rangle \rightarrow |1s,2p^-;s\rangle$ transition energy. Notice that their experimental results were obtained by subtracting the electron cyclotron energy $\hbar\omega_c$ from the measured values of the $|1s,1s;s\rangle \rightarrow |1s,2p^+;s\rangle$ transition energy. The validity of this procedure was checked in Refs. 21 and 10 for a thick-barrier superlattice case. In our calculation, we have included (1) the structure of the superlattice, (2) the polaron correction, and (3) the effect of band nonparabolicity. We found that agreement between theory and experiment is reasonable, especially at high-magnetic fields. The corresponding results for the case of a QW with $w = 95$ Å, 194 Å, and 373 Å without any polaron and band nonparabolicity corrections are also plotted as the open circles for comparison, which were calculated by Huant *et al.* using the variational quantum Monte Carlo method.[22] Notice that the transition energy increases with both decreasing well width and increasing magnetic field. The experiment indicates that the superlattice with the smallest well width, $w = 58$ Å, shows the weakest magnetic-field dependence, and its slope is similar to the results as for the superlattice with $w = 373$ Å. This is opposite to the general trend of increasing slope of the curves with both increasing magnetic fields and decreasing well width w, which was found theoretically and experimentally for $w > 90$ Å.

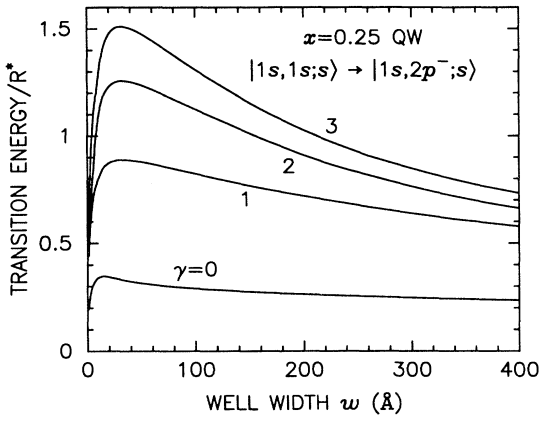

FIG. 9. The transition energy between the ground state and the lowest singlet excited state of a D^- center in a $GaAs/Al_{0.25}Ga_{0.75}As$ QW as function of the well width for four values of the magnetic field: $\gamma = 0$, 1, 2, and 3.

In order to understand this we plot in Fig. 9 the same transition energies, but without the polaron and band nonparabolicity corrections, as a function of well width for a $GaAs/Al_{0.25}Ga_{0.75}As$ QW for the magnetic fields: $\gamma = 0$, 1, 2, and 3. Notice that (i) the transition energy has a stronger well-width dependence at high-magnetic field than at low-magnetic field. This explains why the transition energies from the different superlattices in Fig. 8 are closer to each other in energy in low-magnetic fields than in high magnetic fields; (ii) for a QW with $w >$ 25 Å a decrease of the transition energy becomes more

rapid with decreasing magnetic field, and the smaller the well width, the stronger the magnetic-field dependence. From these observations it is difficult to understand the experimental data for the $w = 58$ Å superlattice, and they require further study.

V. DISCUSSION AND CONCLUSION

We have investigated the energy levels of a D^- center which is located at the well center of a GaAs/Al_xGa_{1-x}As superlattice in the presence of a magnetic field which is directed along the growth axis. The binding energy and the transition energy of the D^- center have been obtained as function of the magnetic field and the well width. A detailed comparison between the results (1) of a QW and a superlattice and (2) with and without e-e correlation terms has been performed. This showed that the structure of the Q2D systems (QW versus superlattice) strongly influences the binding energy of the D^- center, and e-e correlation is essential in the calculation for the D^- states. The correlation contribution to the energy of the D^- center is discussed in detail, and shown to be more important for the excited states and at small magnetic fields. The electron-phonon interaction is included in our calculation within second-order perturbation theory, which shifts the energy levels to lower energies, and leads to resonant splitting of the energy levels at high magnetic fields. In high magnetic fields, i.e., $\gamma > 1.5$, the effect of band nonparabolicity is important. Our theory, which contains *no* fitting parameters, is in good agreement with most of the available experimental data. We found that the experimental results of Huant *et al.*[21] cannot be interpreted as being the *binding* energy of the D^- center. They should be interpreted as the *transition* energy between two D^- states.

Recently, Chang *et al.*[52] have studied the magnetic-field dependence of the binding energy of the D^- center at the well center of an $x = 0.3$, $w = 210$ Å, and $b = 150$ Å superlattice using temperature dependent magnetotransport measurement. They found that the experimental results are systematically smaller in energy than those from the optical transition measurement, and are found to be consistent with the theoretical calculation of Pang and Louie.[26] However, we have noticed in the present paper that the electron-phonon interaction is a very important effect on D^- centers in polar materials, which was neglected in Ref. 26. This effect will greatly increase the binding energy of the D^- center to a level higher than the corresponding transition energy. Thus, these alternative experimental data need further theoretical study.

ACKNOWLEDGMENTS

One of us (F.M.P.) is supported by the Belgian National Science Foundation. J.M.S. wishes to thank Technology University Eindhoven for financial support. We are grateful to S. Huant, B.D. McCombe, and J.P. Cheng for providing us with their experimental data. This work is sponsored by "Diensten voor de Programmatie van het Wetenschapsbeleid" (Belgium) under Contract No. IT/SC/24 and the Fonds voor Kollektief Fundamenteel Onderzoek, Belgium, Project No. 2.0093.91.

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